Dynamic FT-IR Analysis of Polymers

using continuous scan, dual channel data acquisition

USER

MANUAL

BRUKER *Optics*

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1. Safety Advice

If the Polymer Modulator[TM] by Manning Applied Technology was part of your delivery, please follow the safety warnings and instructions given in the related manual from Manning Applied technology. If you use a polymer stretcher of an other manufacturer, please consult the respective manual for safety advice.

In the appendix of this document, the most important warning labels and the adequate precautions are listed.

2. Introduction

Applying dynamic strain on polymers (or related materials) combined with phase-sensitive FT-IR spectroscopy, provides insight into the dynamic behavior and flexibility of these materials. Besides the general interest in the in-phase and out-of-phase spectra, measurement series (e.g. with different modulation frequencies or polarization angles) can be of further help to gain access to relevant data concerning the dynamic behavior of the investigated molecules.

Compared to earlier approaches based on the Step-Scan technology using so-called amplitude modulation, the dual channel acquisition technique, described in this manual, is clearly superior. In an amplitude-modulated Step-Scan experiment, a considerable fraction of the total measurement duration is used for accelerating, stopping and repositioning of the interferometer mirror. During this time, no data is acquired, making the Step-Scan approach a rather inefficient one. By contrast, the dual channel technique uses the measurement time much more efficiently. Furthermore, the dual channel acquisition technique is also superior to the so-called multiplexing technique which, for example, reduces the accessible spectral bandwidth and in some cases might degrade the signal quality.

Modern Bruker Optics research FT-IR spectrometers are equipped with a 2-channel 24bit ADC (**A**nalog to **D**igital **C**onverter) which is integrated in the detector socket (so-called Digitect^{TM} technology), allowing for acquisition of all DMA relevant data while the interferometer mirror is continuously moving. One channel of the ADC is used for recording and digitizing the repeated interferograms which are separated by constant time intervals. Simultaneously, the second ADC channel records and digitizes the time-dependent strain data of the polymer stretcher. As soon as such a measurement is finished, the in-phase and the out-of-phase spectra can be extracted using a smart software algorithm which is part of the OPUS^{TM} software (version 6.0 or higher). For a given measurement duration, the S/N (**S**ignal to **N**oise ratio) of the dual channel technique will be distinctly superior, compared with a Step-Scan measurement.

3. Technical Requirements, Sample Preparation and Installation

3.1 Required hardware

- FT-IR spectrometer with highly sensitive Digitect^{TM} detector (e.g. MCT or InSb) including a 2-channel ADC with activated second channel. A detector prepared for using the 2nd channel is easily recognized by the two cables coming out at the rear side of the detector socket (fig. 1).

Fig.1: Rear side of a Digitect^{TM} detector with activated 2nd channel (in this example an MCT detector). The dual channel ability is indicated by the two additional cables led out from the detector socket.

- Polymer stretcher (with controller) installed in the sample compartment.

- Frequency generator with frequency range of approx. 0-70Hz and sinusoidal output voltage of 5V (peak to peak) in order to reach the full amplitude of the polymer stretcher.

- Recommended: polarizer for polarization-dependent measurements.

- Remark: Using an additional optical band-pass or low-pass filter can distinctly improve the signal to noise ratio. In this manner, parts of the irrelevant spectral range can be blocked allowing the usage of a larger spectrometer aperture which in turn increases the S/N in the spectral range of interest.

3.2 Required software

- For data evaluation, the DMA algorithm is essential. Therefore, OPUS version 6 (or higher) is required. For data acquisition and data visualization, the packages OPUS/CHROM and OPUS/3D are absolutely necessary.

3.3 Sample preparation

- The foil, you intended to analyze, should be rectangular in shape with a width of approximately 25mm and a height of 10 to 45mm. Experience shows that a roughly quadratic shape (25x25mm^2) is preferable.

- In order to avoid undesired multiple beam interferences, roughen one side of the foil with abrasive paper.

- The two edges of the foil which are to be clamped into the polymer stretcher should be masked from both sides with paper (or carton etc.). This measure ensures a uniformly oscillating strain of the foil during the experiment and prevents the sample edges from slipping out of the mount. A convenient way for preparing the sample is, for example, masking the sample edges with approximately 5mm wide stripes of so-called "post-it®" paper (used in many offices) which has an adhesive area on one side (fig. 2).
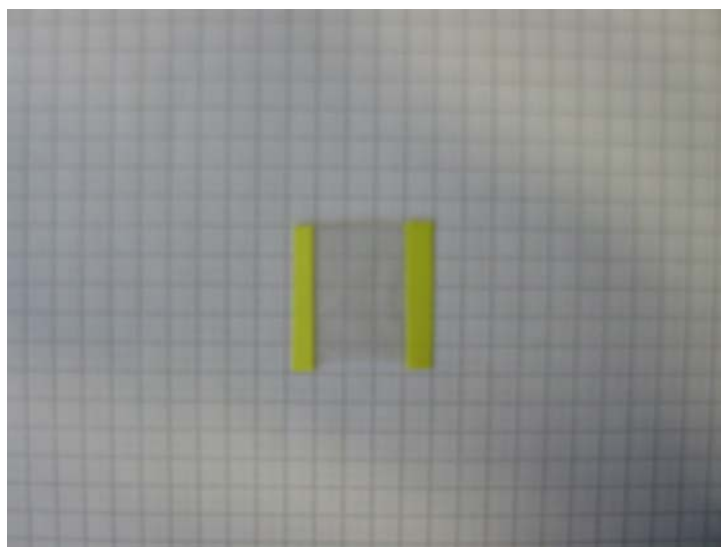
Fig. 2: Prepared polymer sample (isotactic polypropylene) with its edges covered by so-called "post-it®" paper. The squares in the background have a side length of 5mm.

3.4 Installation

This manual describes only the installation using the Polymer Modulator™ by Manning technology.

- Cool the detector by filling liquid nitrogen into the detector dewar.

- Start the *OPUS* software.

- Mount the sample into the clamping jaws of the polymer stretcher. Ensure that the sample is mounted symmetrically. (See fig. 3.) Slightly stretch the sample using the micrometer screw. The sample is correctly mounted if it has no crinkles. Put the polymer stretcher into the sample compartment of the spectrometer. If you want to measure with a polarizer and/or an optical filter, put it into the mount on right hand side of the polymer stretcher.

- Connect the controlling unit of the Polymer Modulator™ to power supply, but still keep it turned off. Turn the bias and the gain control knobs fully to the left (minimum position). Connect the polymer stretcher and the controlling unit (panel location labeled "HEAD") using the thick cable which is included in the Polymer Modulator™ package.

**Fig. 3:** Polymer stretcher with correctly mounted polymer sample.

- Connect the frequency generator to the power supply and turn it on. Choose a sinusoidal output and adjust the voltage amplitude to a value below but close to 5V (peak to peak). Then, adjust the generator to the desired modulation frequency. A commonly used frequency is 18Hz, however, other frequencies can be of interest as well. In the first few minutes after adjusting the frequency, many frequency generators tend to drift slightly (typically in the 2nd decimal place). Before starting a real measurement, always make sure that the displayed frequency does not change anymore. Connect the output of the frequency generator with the BNC connector labeled "INPUT" of the polymer modulator controlling unit using a BNC cable.

- Connect the controlling unit BNC output labeled "STRAIN" with the 2nd channel Input of the detector (typically labeled "from LIA"). An adequate cable (BNC plug at one end, SMB plug at the other end) is included in the delivery. Turn on the controlling unit of the polymer stretcher.

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4. Parameter Setting and Measurement

4.1 Measurement parameters

- Select in the OPUS "Measure" menu the "Chromatography" function. Thereupon, the "Chromatography GC/LC/TGA" dialog window appears. (See fig.4.)
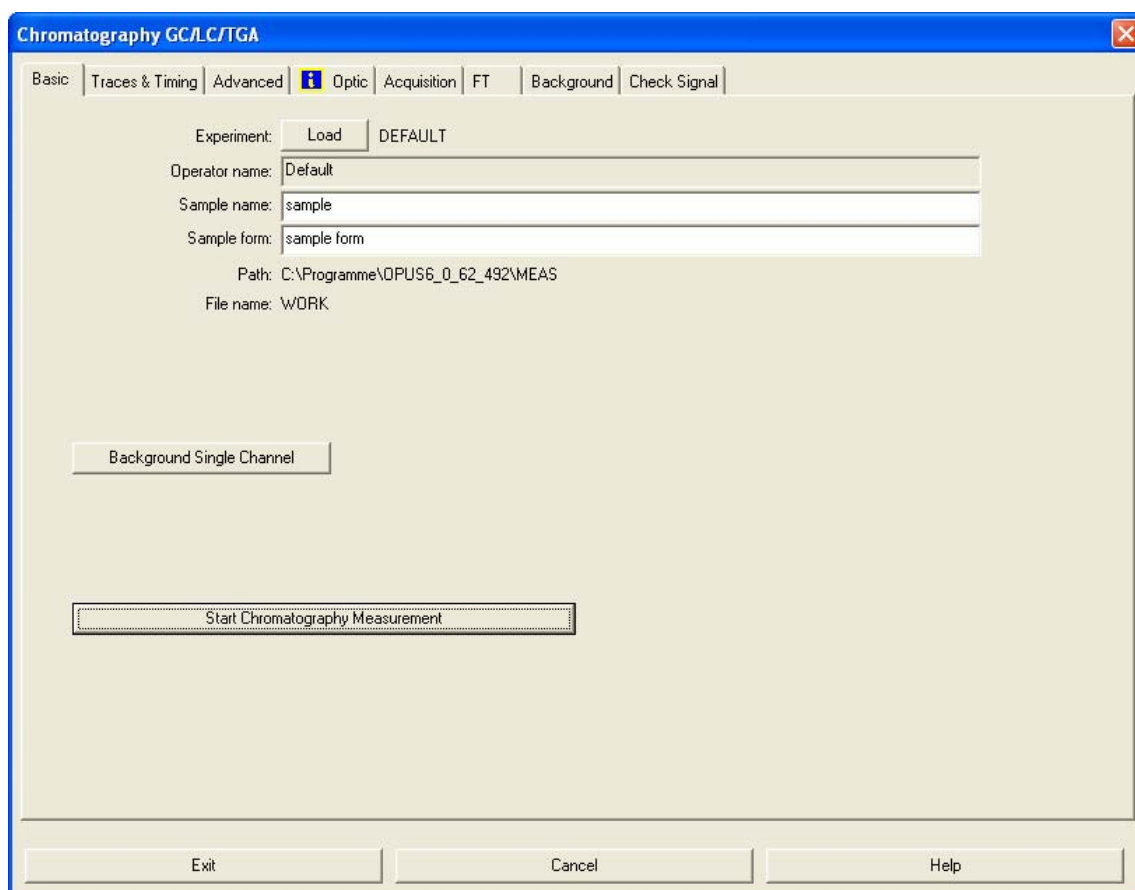
Fig. 4: Chromatography dialog window – Basic page

- On the "Basic" page, you can store additional information such as sample name, sample form etc. On this page, you also start the measurement after having entered all relevant parameters.

- Click on the "Traces & Timing" tab. (See fig.5.) Make sure that the check boxes "Compute Gram Schmid" and "Traces by spectral integration" are not activated because they are only useful for real chromatography measurements. In the group field "Time base synchronization", activate the option button "Off". Activate "Maximum measurement time" check box and enter the desired maximum measurement time. A maximum measurement time of 5 minutes is a good starting point, but depending on the results, you can also test longer and/or shorter measurement times. In the "Save Spectra" drop-down list, it is recommended to select the option "On".
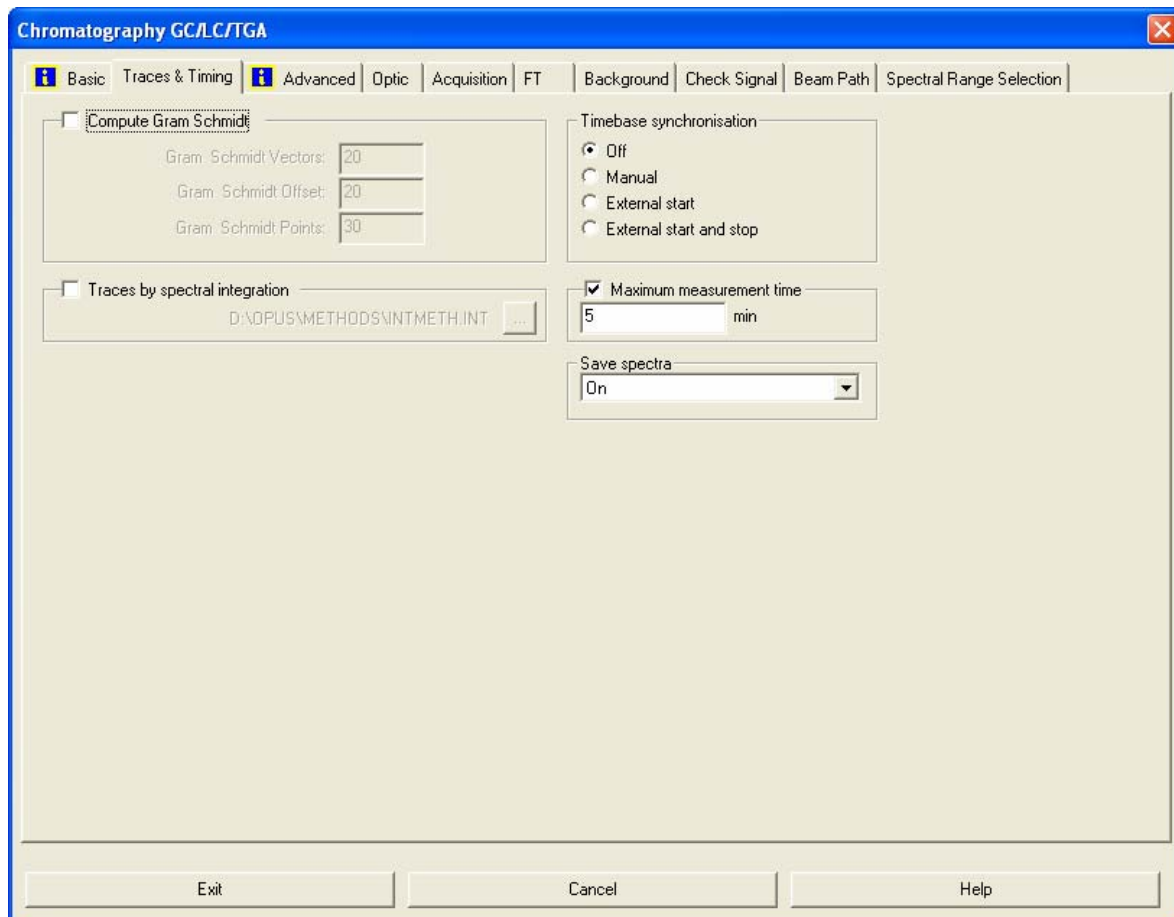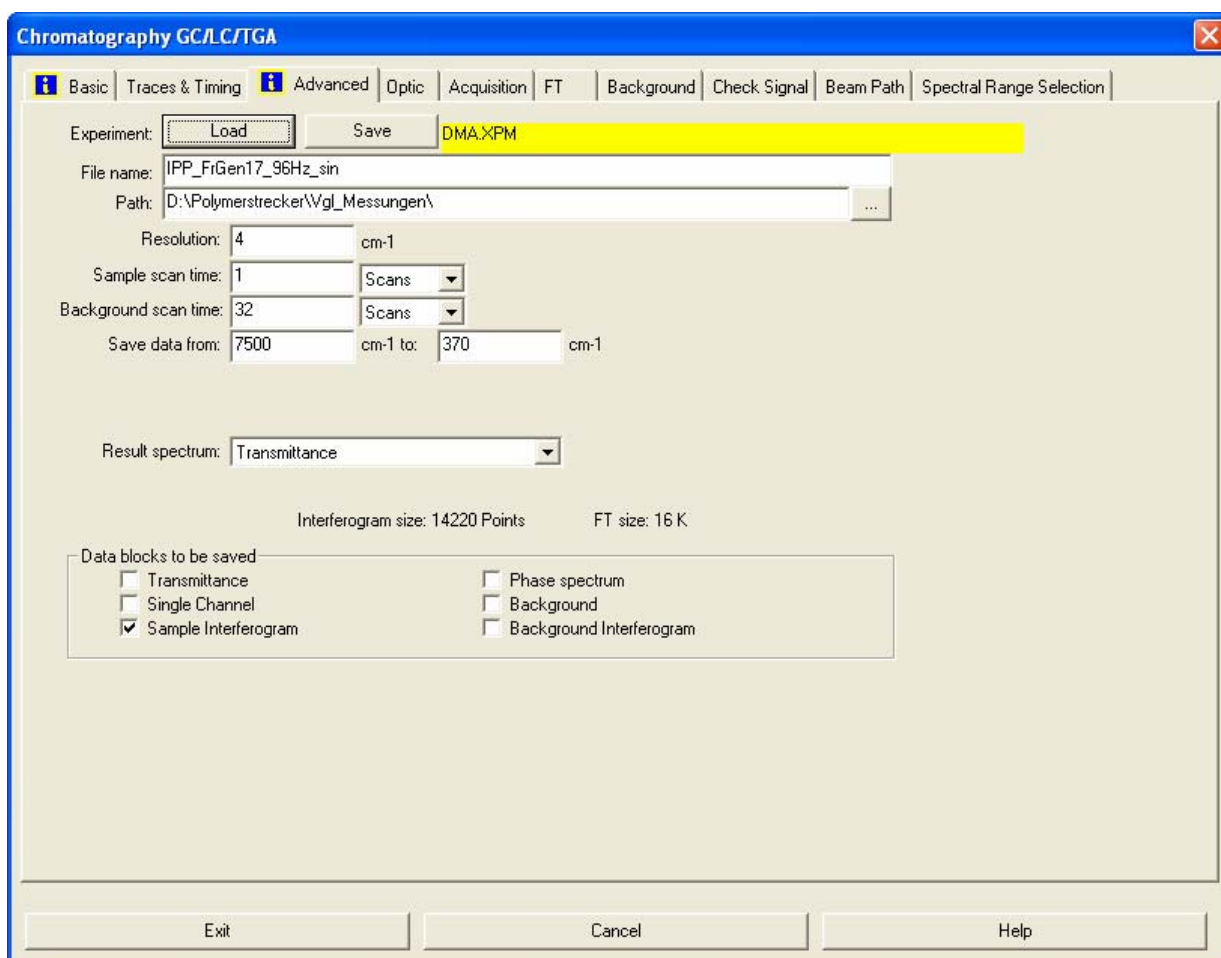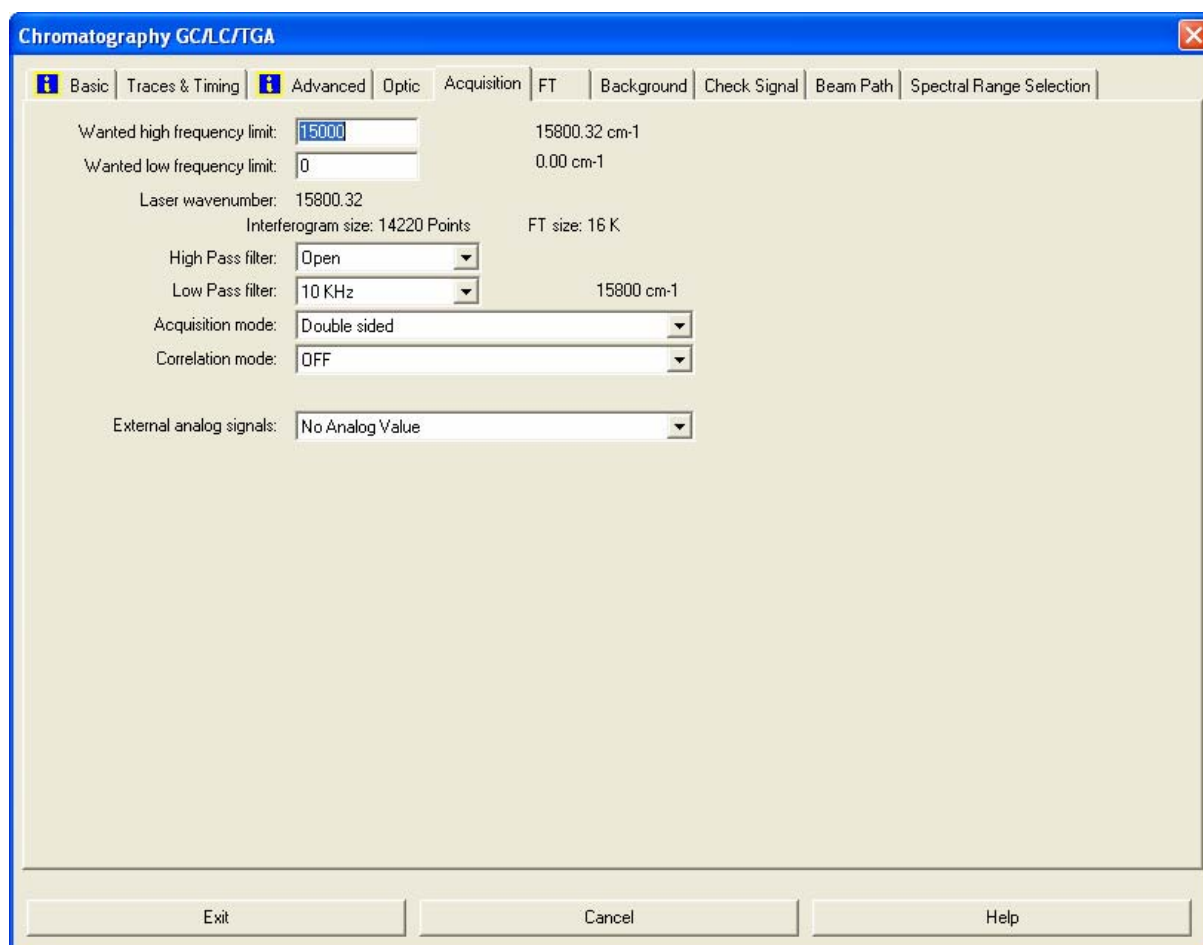
Fig. 5: Chromatography dialog window – Traces & Time page

- Click on the "Advanced" tab. (See fig. 6.) This page is identical to the "Advanced" page of the "Measurement" dialog you probably know from standard FT-IR experiments (e.g. transmittance, reflectance).

- By clicking on the "Load" button, you can load an existing .XPM file that contains parameters which might turn out to be useful for your particular experiment. By clicking on the "Save" button, you can save the measurement parameters you have specified into a new .XPM file for future use. Furthermore, you can enter a "File name" for the measurement results and specify the "Path" under which this file is to be stored.

- For typical polymer stretching experiments, a "resolution" of 4cm^{-1} is appropriate, but you are free to enter a different resolution value. The parameter "Sample scan time", however, MUST be set to 1 scan. Otherwise, the experiment will not work properly. The parameter "Background scan time" is not relevant because the polymer stretching experiment does not require a classical background measurement. In the fields "Save data from…to…" you need not enter anything as well, since the Fourier transformation will be performed later by the DMA algorithm.

- Select in the "Result spectrum" drop-down list the option "Transmittance". In the group field "Data blocks to be saved" activate only the "Sample Interferogram" check box.

Fig. 6: Chromatography dialog window – Advanced page

- Click on the "Acquisition" tab (fig.7). This page is identical to the "Acquisition" page of the standard "Measurement" dialog window. (For detailed information about this dialog window refer to the OPUS Reference Manual). Set the "Wanted high frequency limit" to $15000cm^{-1}$ and the "Wanted low frequency limit" to $0cm^{-1}$. The "High Pass Filter" must always be set to "open". For the "Low Pass Filter", depending on the chosen scanner velocity (see "Optic" page), other settings might be useful as well. For the parameter "Correlation mode", select the option "Off" and for the parameter "External analog signals" always select the option "No Analog Value".

- In case of a polymer stretching experiment, the parameters on the pages "FT", "Background", "Beam Path" and "Spectral Range Selection" need not to be specified.

Fig. 7: Chromatography dialog window – Acquisition page

- Click on the "Optic" tab. (See fig.8.) This page is identical to the "Optic" page of the standard "Measurement" dialog window. The parameters on this page are in both cases the same. (For detailed information about these parameters refer to the OPUS Reference Manual.) Set the following parameter values:

      External synchronization: Off
      Optical Filter setting: Open
      Source setting: MIR (in most cases)
      Beamsplitter: KBr (in most cases)
      Measurement channel: Sample compartment
      Sample signal gain: x1
      Background signal gain: x1
      Preamp gain: Ref
      Scanner velocities: Recommended values are 5, 10 or 20kHz.

The list "Detector settings" includes 3 options for the MCT detector with the activated 2nd channel. (See fig. 8.) Each detector channel can be accessed separately, or both of them simultaneously. The syntax of these entries is as follows:

detector type   channel information   [detector position]

The detector with the activated 2nd channel is "LN-MCT Mid". (See fig. 8.) This detector is mounted in the internal detector position no.2 of the spectrometer. Therefore, each of the 3 entries ends with "[Internal Pos.2]".

1st ADC-channel: The option for the detector with the first activated ADC-channel does not include any channel information. This channel records the standard infrared signal (interferogram). For this case, it is the option "LN-MCT Mid [Internal Pos.2]".

2nd ADC-channel: The option for the detector with the second activated ADC-channel includes as additional channel information "External Sig." (in some cases "demodulated"). This channel records the strain signal of the polymer stretcher. For this case, it is the option "LN-MCT Mid External Sig. [Internal Pos.2]".

Dual channel acquisition: For a measurement with both channels, select the option which contains "plus…" as additional channel information.
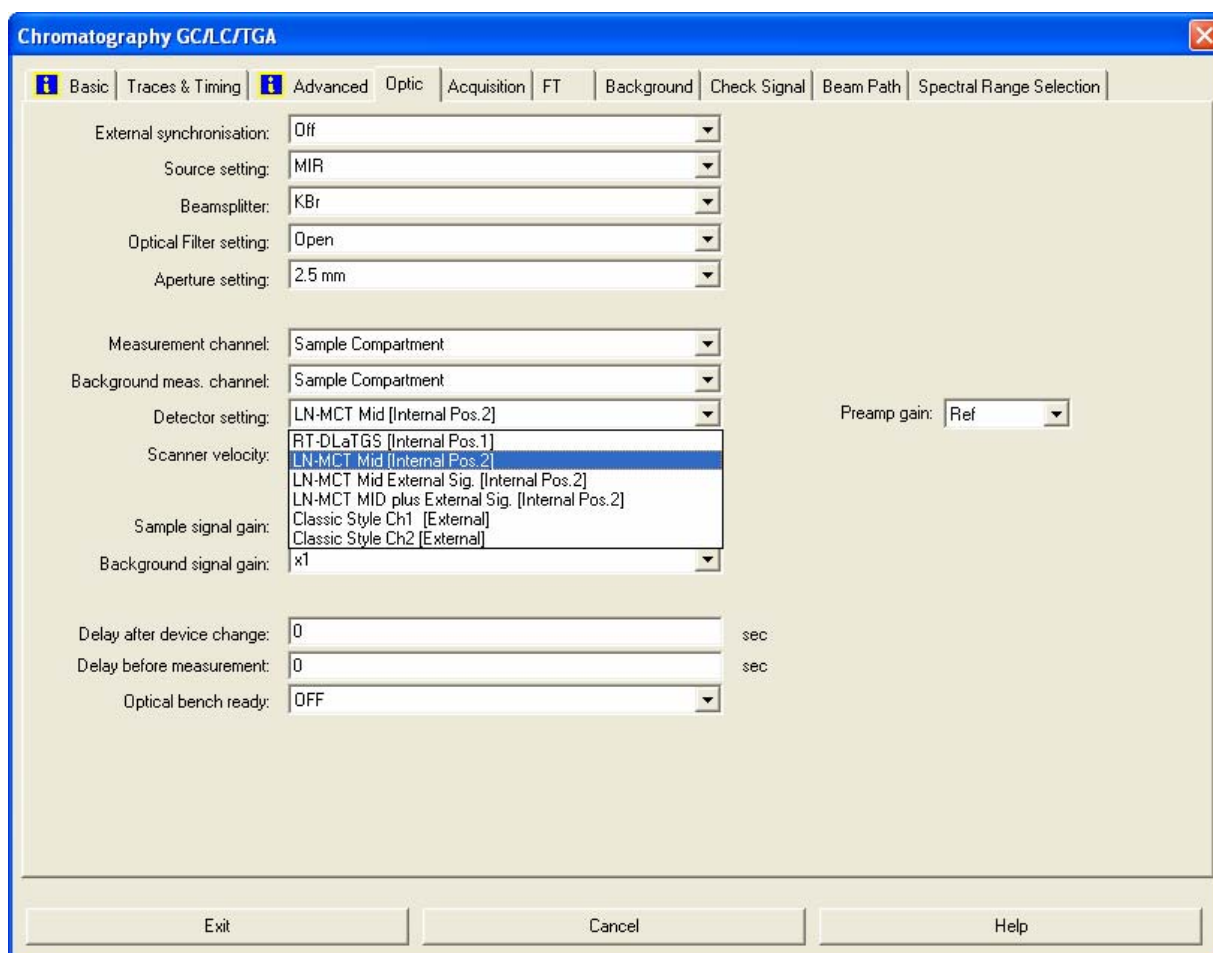
**Fig. 8:** Chromatography dialog window – Optic page showing the available detector options

- Select the option "LN-MCT Mid [Internal Pos.2]" (i.e. MCT detector with 1st activated ADC-channel) and click on the "Check Signal" tab (fig.9) in order to check the infrared signal. Depending on the displayed signal level, you can increase or decrease the "Aperture Setting" on the "Optics" page. In principle a higher signal level will always result in a better signal/noise ratio (S/N), but avoid to get too close to detector saturation.

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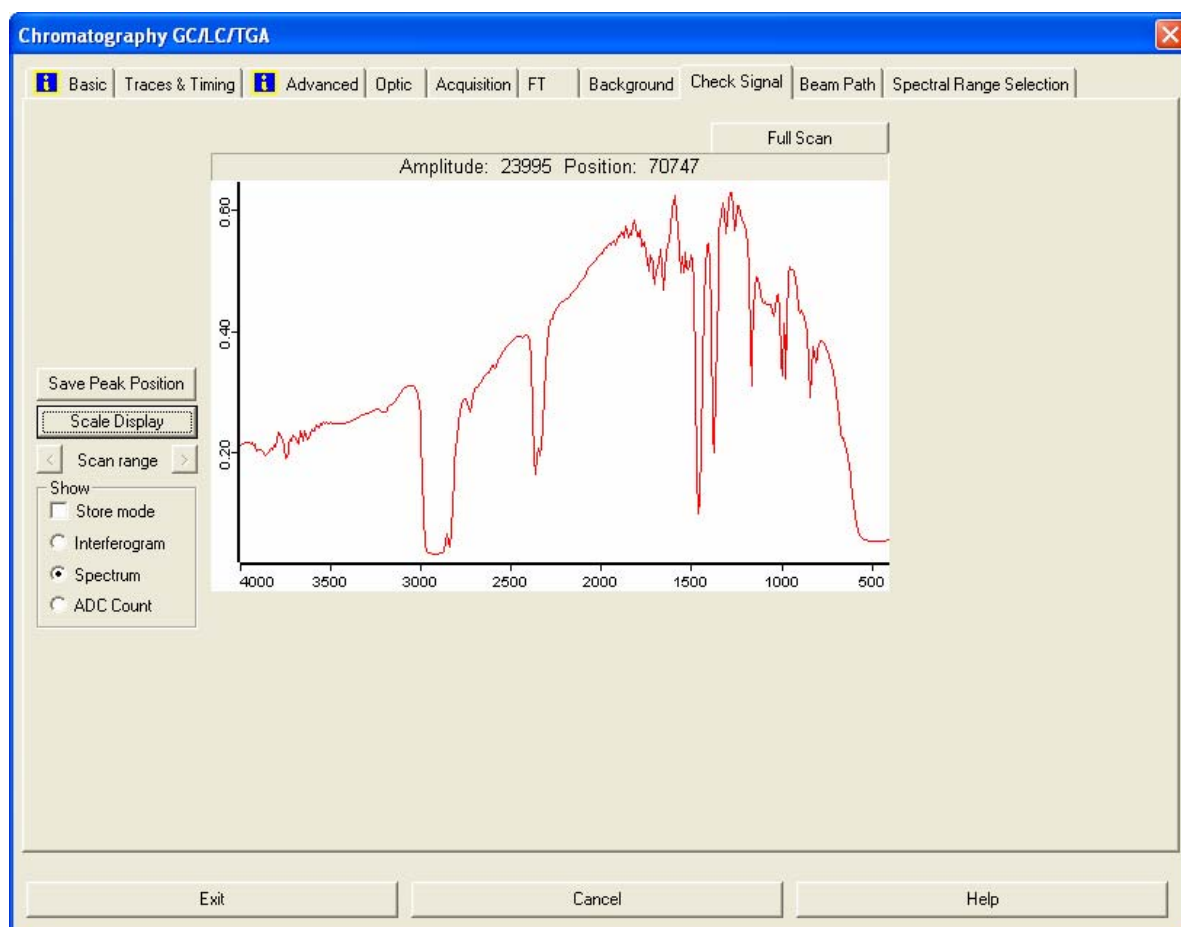
Fig. 9: Chromatography dialog window – Check Signal page showing the infrared signal (spectrum or interferogram) detected by the MCT detector with first ADC channel.

- Select the option "LN-MCT Mid External Sig. [Internal Pos.2]" (i.e. MCT detector with 2nd activated ADC-channel) and click on the "Check Signal" tab in order to check the strain signal (stretching amplitude) of the polymer stretcher. (See fig.10.) Slowly increase the "GAIN" of the polymer stretcher controlling unit by turning the knob to the right until the strain signal of the stretcher is sinusoidal. While the "GAIN" knob controls the amplitude of the strain signal, the "BIAS" knob controls the offset. By using these two controlling knobs, maximize the sinusoidal signal, but avoid in any case that the top or the bottom of the signal are clipped (flattened). This procedure is described more detailed in the Polymer Modulator™ manual provided by Manning Applied Technology.

- Also check whether the stress of the sample is correctly adjusted. To do this, remove the cable of the 2nd ADC channel from the "STRAIN" BNC output of the controlling unit and plug it into the "STRESS" BNC output. On the "Check signal" page, once again a sinusoidal signal is displayed, which usually contains more noise and is weaker in intensity compared to the strain signal. (See fig. 11.) To optimize the stress signal, carefully adjust the micrometer screw of the polymer stretcher. The sample stress is one of the most crucial parameters in the whole experiment: too low as well as too high stress may lead to bad results. Therefore, it is recommended to run the experiment with different stresses and find out the best adjustment for your particular sample.

- **Note:** The "STRAIN" and the "STRESS" signal can be alternatively checked with an oscilloscope.

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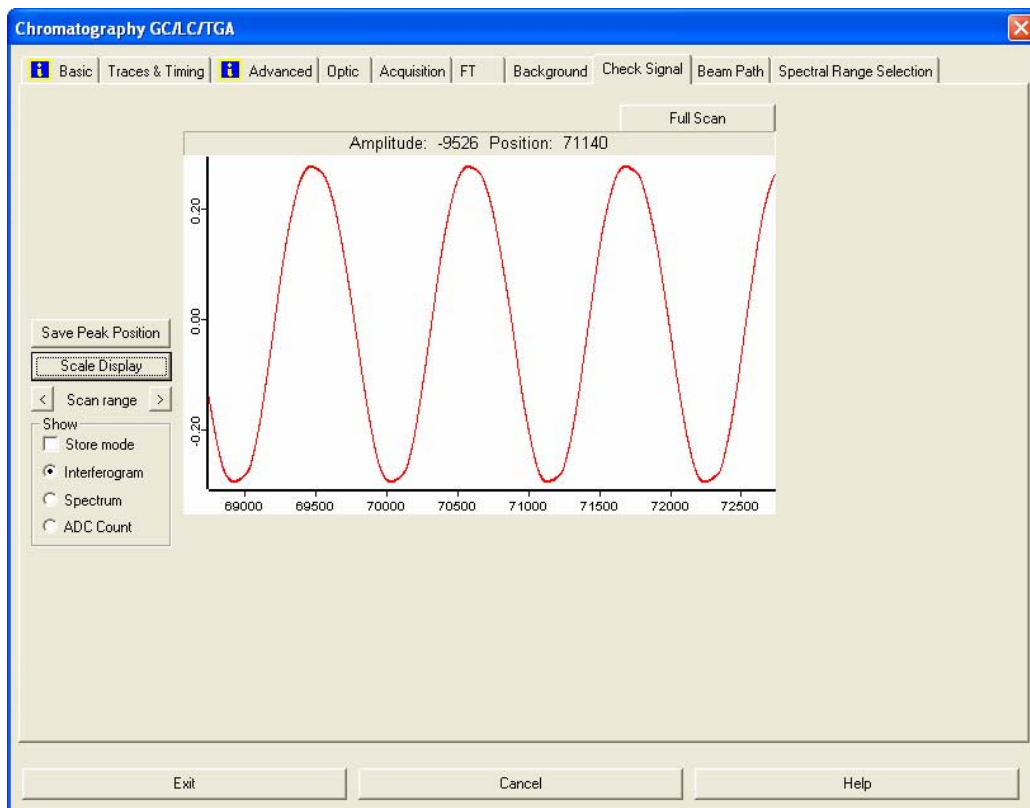
Fig. 10: "Check Signal" page displaying the correctly adjusted strain signal (using the 2nd ADC channel). The signal is maximized and neither the top nor the bottom of the sinusoidal signal is clipped. Note: It is normal that the strain signal moves along the X-axis when it is displayed on the "Check Signal" page.
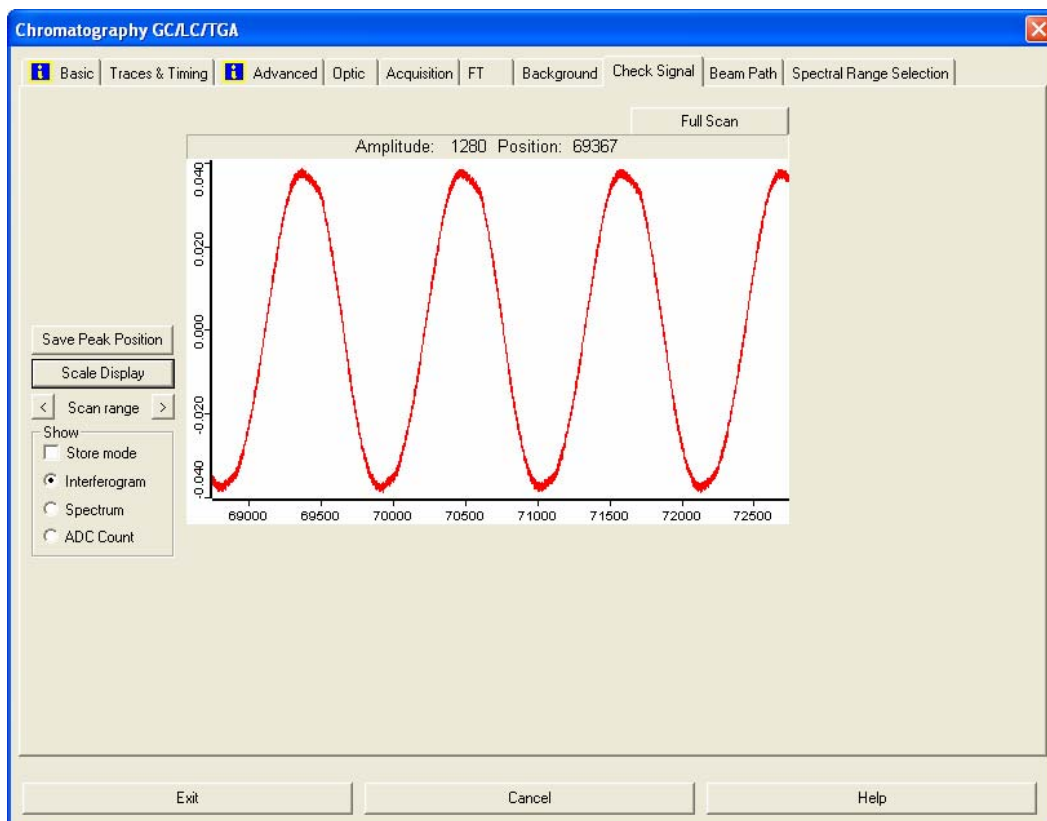
Fig. 11: "Check signal" page displaying the stress signal (using the 2nd ADC channel). This signal is more noisy and weaker in intensity compared to the strain signal, but it is still sinusoidal.

4.2 Sample measurement

- Plug the cable of the 2nd ADC channel into the "STRAIN" output of the controlling unit again. Click on the "Optic" tab and select the detector option "LN-MCT MID plus External Sig. [Internal Pos.2]" (i.e. the MCT detector option that allows measurements with both ADC channels). Finally, start the measurement by clicking on the "Basic" tab and afterwards on the "Start Chromatography Measurement" button.

- The measurement result is stored in a dual channel 3D file. The 3D block named "S_IFG", contains all the single interferograms and the 3D block named "2_chn" contains all the single strain traces. Double-clicking on the "S_IFG" data block in the OPUS browser opens a 3D+ window in which the single interferograms are displayed in a 3D plot (left upper subwindow). See figure 12. (The file containing the measurement results is called "ipp.0" because the sample is isotactic polypropylene.)
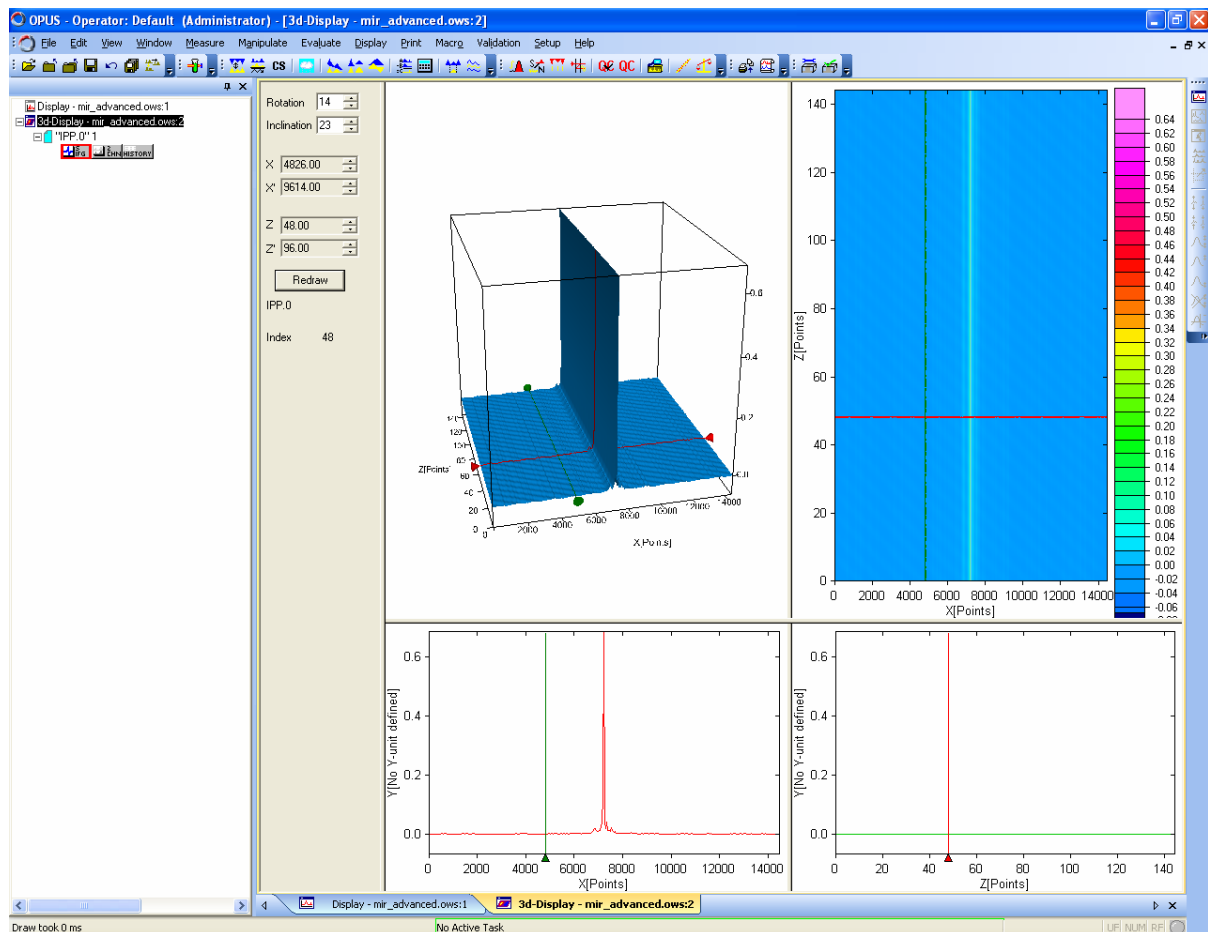
Fig. 12: OPUS 3D+ window - In the 3D plot (left upper subwindow) all the single interferograms acquired with the first ADC channel of the detector are displayed. These interferograms are in the "S_IFG" data block of the 3D file.

- Double-clicking on the "2_chn" data block in the OPUS browser opens a 3D+ window in which the single strain traces are displayed in a 3D plot (left upper subwindow). See figure 13. These strain traces have been acquired simultaneously with the interferograms shown in figure 12. For the DMA algorithm, which will be used for evaluation, it is extremely important that there is a certain phase shift of the strain signal for consecutive interferograms. To find out whether there is a phase shift, have a look a the contour plot in the right upper subwindow of the 3D+ window that shows parallel lines (minima

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and maxima of the strain signal). See figure 13. (Note: If this is not the case, it might be necessary to adjust the contour level color scale. For detailed information about the 3D+ window refer to the OPUS/3D Manual.) If there is a phase shift between two consecutive interferograms (scans) the parallel lines incline as indicated by the angle α in figure13. The angle should not be too small. It depends on the relation of scanner velocity, resolution and modulation frequency. Thus, this angle can be influenced by changing one or several of these parameters. Estimate the number of modulation periods along the x-axis of the contour plot. (xz-plot). The number of periods along the **z**-axis should be at least equal to the number of periods along the x-axis or even larger. In case of the example shown in figure 13, there are approximately 2 times more periods along the z-axis than along the x-axis.
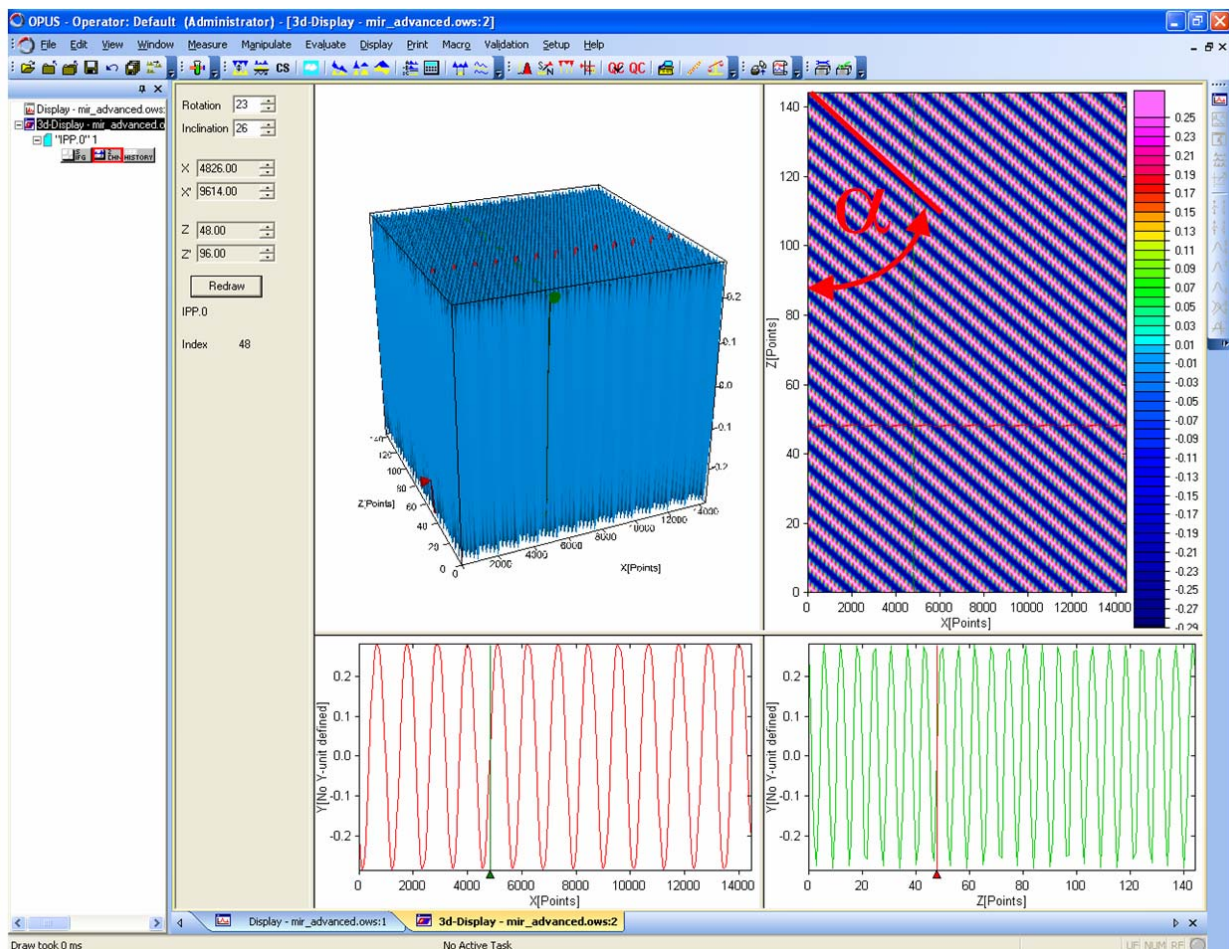

Fig. 13: OPUS 3D+ window - In the 3D plot (left upper subwindow), all the single strain traces acquired with the second ADC channel of the detector are displayed. The strain traces are in the "2_chn" data block of the 3D file. On the basis of the contour plot in the right upper subwindow, you can assess the phase shift of the strain signal by the inclination of the parallel lines (indicated by the angle α).

4.3 Calibration measurement

Hint: Before you remove the sample in order to start the calibration measurement, it is recommended to repeat the sample measurement with slightly different stresses. The stress can be adjusted using the micrometer screw.

-   Turn off the controlling unit of the polymer stretcher. Remove the sample and mount the shutter aperture (which is included in the delivery) into the moving jaw of the polymer stretcher. Mount it in such a way that roughly half of the

light is blocked. Because without the sample, the light intensity reaching the detector is higher than with sample, so it might be necessary to select in OPUS a smaller aperture setting. Change the file name in such a way that the file can easily be recognized as the file containing the calibration measurement results. All the other parameter settings should be identical to the ones of the sample measurement. Turn the controlling unit on again. Then, start a dual channel measurement (i.e. with both ADC channels of the detector) as already described in section *4.2 Sample Measurement*. Because the light intensity has been modulated during the calibration measurement, the inclined lines can now easily be seen in the 3D plot. (See figure 14.) The strain traces of the calibration measurement will look identical to the ones of the sample measurement.
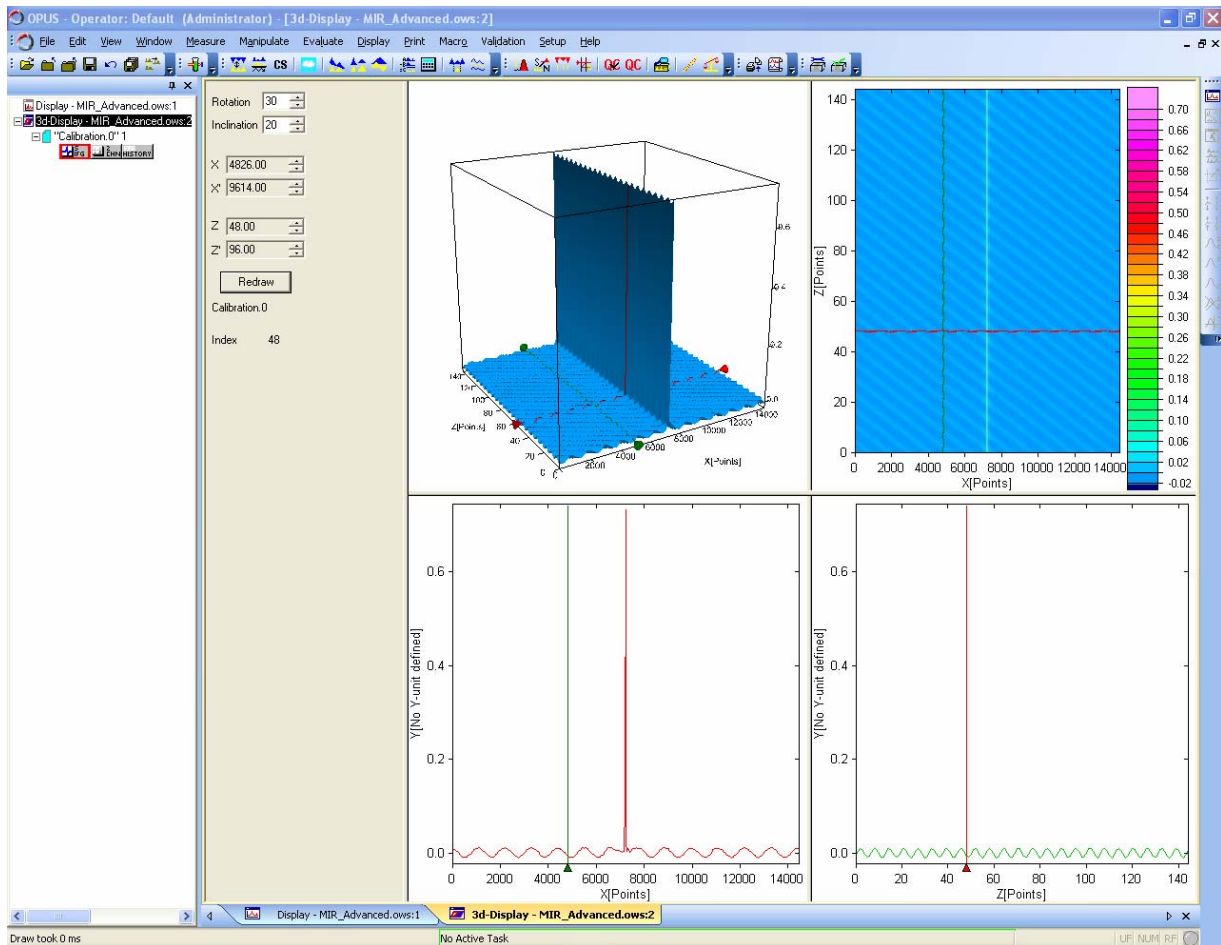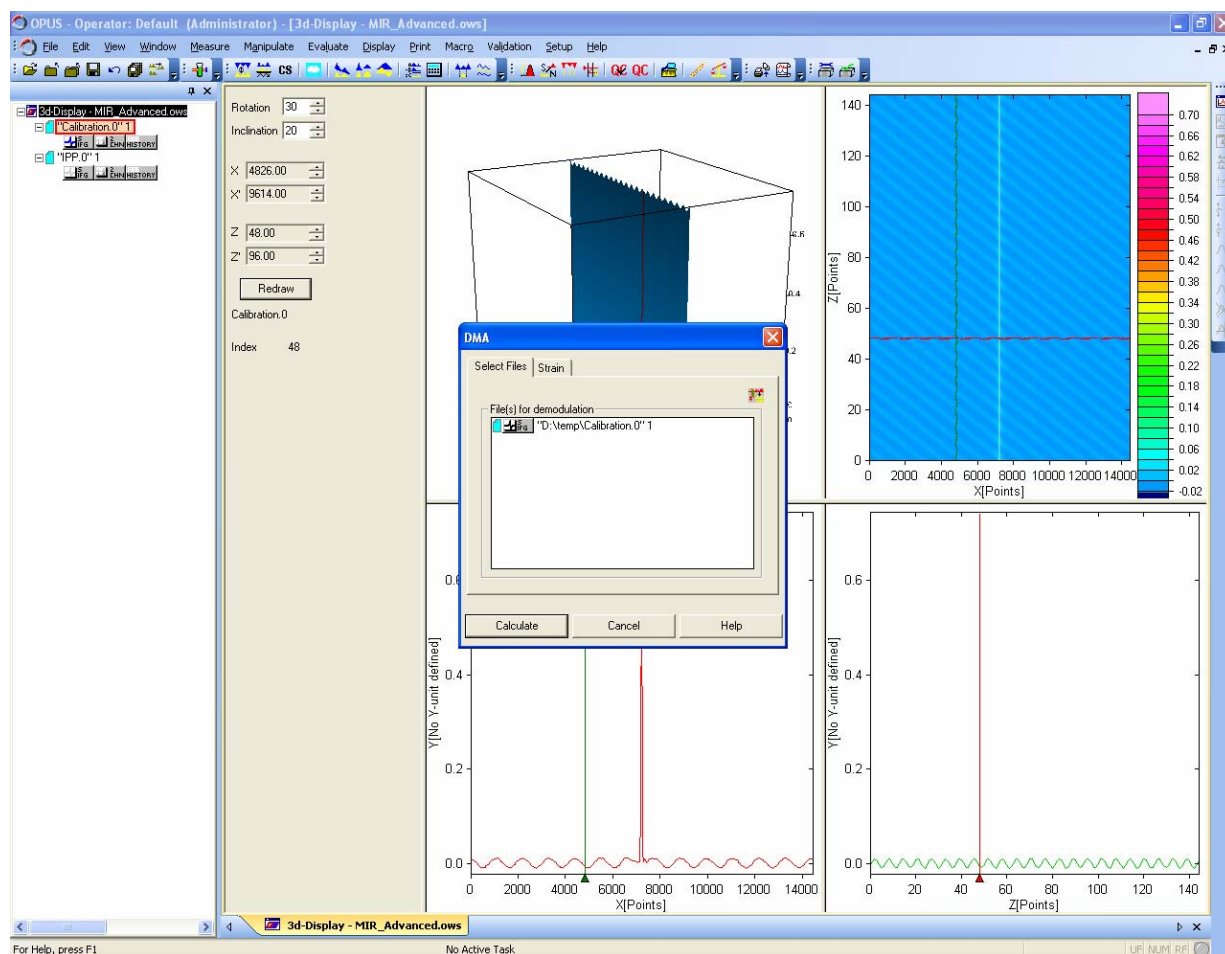

Fig. 14: OPUS 3D+ window displaying the single interferograms of the calibration measurement. (The interferograms are in the "S_IFG" data block of the 3D file resulting from the calibration measurement. These interferograms contain strong modulations due to the oscillating shutter aperture.

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5. Data Processing

5.1 Applying the DMA algorithm to the calibration and sample data

- Select in the OPUS browser the 3D file resulting from the calibration measurement by clicking on it with the left mouse button. Then, select in the "Evaluate" menu the "DMA" function. Thereupon, the "DMA" dialog window appears. (See figure 15.) In the field "File(s) for demodulation ", the data block "S_IFG" resulting from the calibration measurement should already be included. If not, just drag & drop the data block "S_IFG" of the corresponding 3D file into this field.

- Click on the "Strain" tab in the "DMA" dialog window. (See figure 16.) Enter the modulation frequency of the polymer stretcher into the "Frequency" field. In most cases (particular for experiments using the Polymer Modulator^{TM} by Manning Technology), the value for the parameter "Phase" should be "0". Only if you use a modulator of which the strain output has an electronic phase shift with respect to the physical strain, this can be compensated by entering a different parameter value. The remaining parameters on the "Strain" page are not relevant to this kind of experiment. (They are only useful for "old fashioned" step scan or multiplexing based experiments.) Click on the "Calculate" button.


Fig. 15: DMA dialog window - Select files" page. The "S_IFG" data block of the 3D file resulting from the calibration measurement is included.
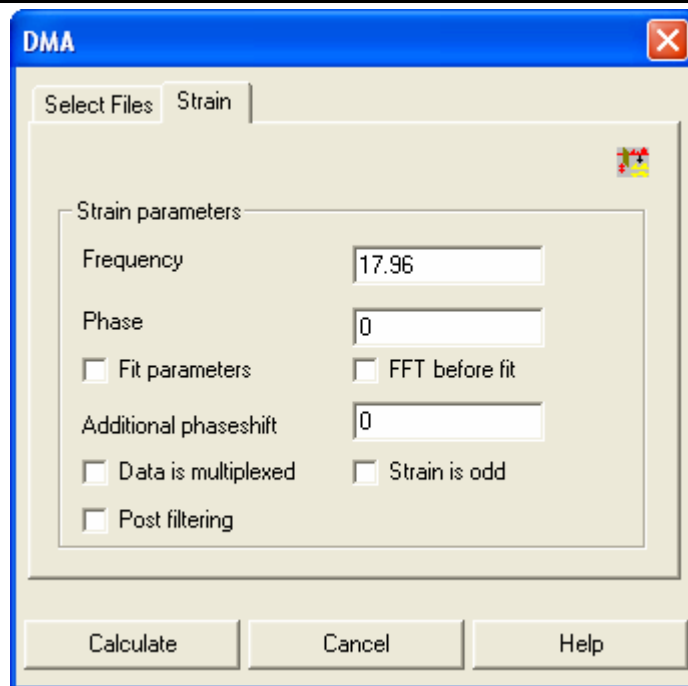
Fig.16: DMA dialog window - Strain" page. Only the parameters "Frequency" and the "Phase" are relevant to this kind of experiment.

The DMA algorithm calculates several new interferograms which are added as additional data blocks to the 3D file in the OPUS browser. See figure 17. The data block **"S_IFG"** is that part of the infrared signal which does not depend on the different strain phases at all. The data blocks **"S_IFG"** and **"2_CHN"** result from the sample measurement which has been performed before the DMA calculation (i.e. these data blocks contain the pure measurement results). The fourth block **"S_IFG^R"** is the real part of the DMA demodulation. It is the part of the infrared signal which is in phase with the strain signal. The fifth block **"S_IFG^I"** is the imaginary part of the DMA demodulation. Its interferogram is 90° phase-shifted with respect to the strain signal. It is also called quadrature interferogram.

Drag & drop the calibration data file in the standard OPUS spectrum window. (See figure 17.)
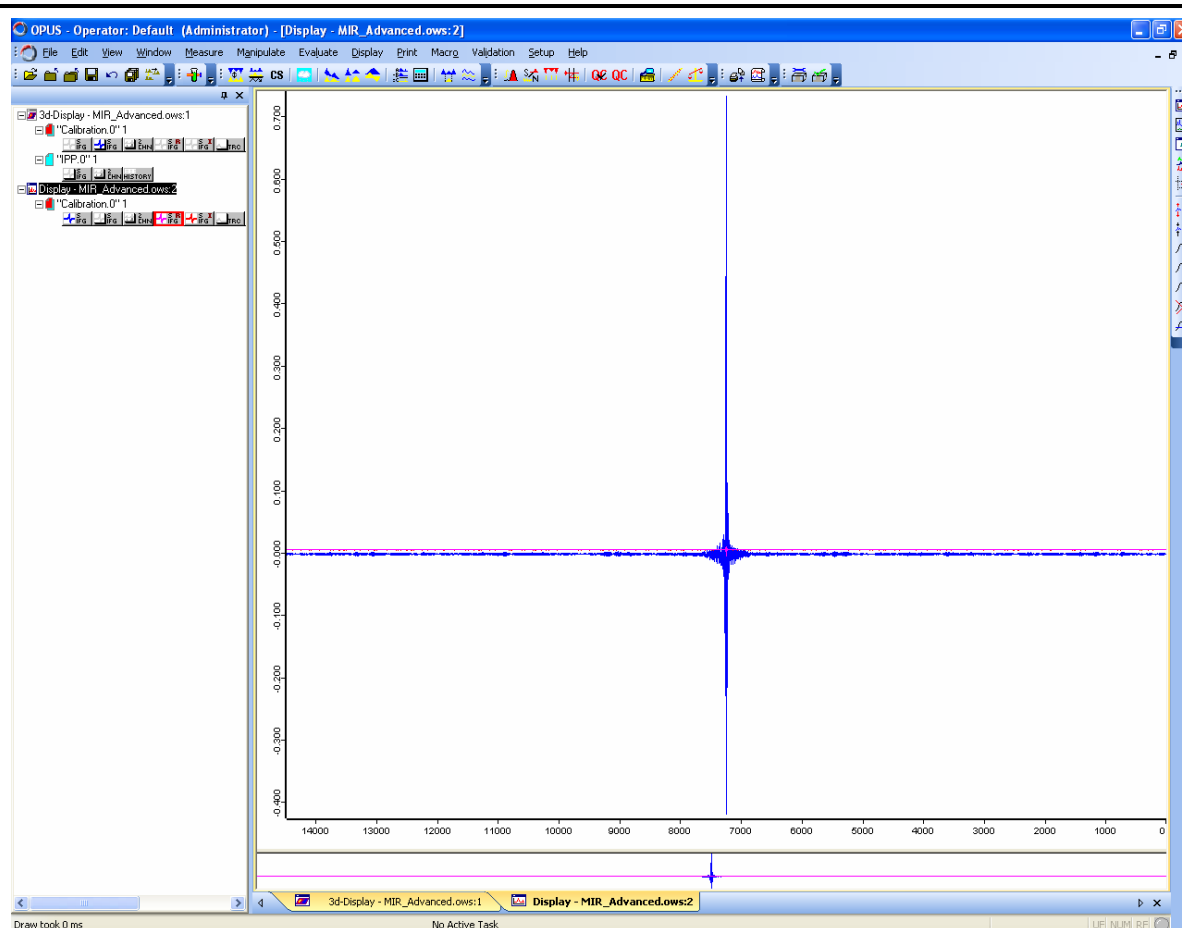
Fig. 17: OPUS browser with the calibration file after the DMA calculation (i.e. several new data blocks have been added to the file).

- Select in the OPUS browser the file resulting from the sample measurement by clicking on it with the left mouse button. Then, select in the "Evaluate" menu the "DMA" function. Apply the DMA function to file resulting from the sample measurement with exactly the same parameter settings as for the file resulting from the calibration measurement. Also in case of the sample measurement file, additional interferogram blocks will be added to the file in the OPUS browser. These blocks have the same meaning as described above for the calibration measurement.

- Drag & drop the file resulting from the sample measurement in the standard OPUS spectrum window (not in a OPUS 3D window).

## 5.2 Extraction of the calibration phase spectrum

- Select the data block "S_IFG^R" (containing the real part interferogram) of file resulting from the calibration measurement. Then, select in the "Manipulate" menu the "Interferogram to Spectrum" function. Thereupon, the dialog window shown in figure 18 appears.

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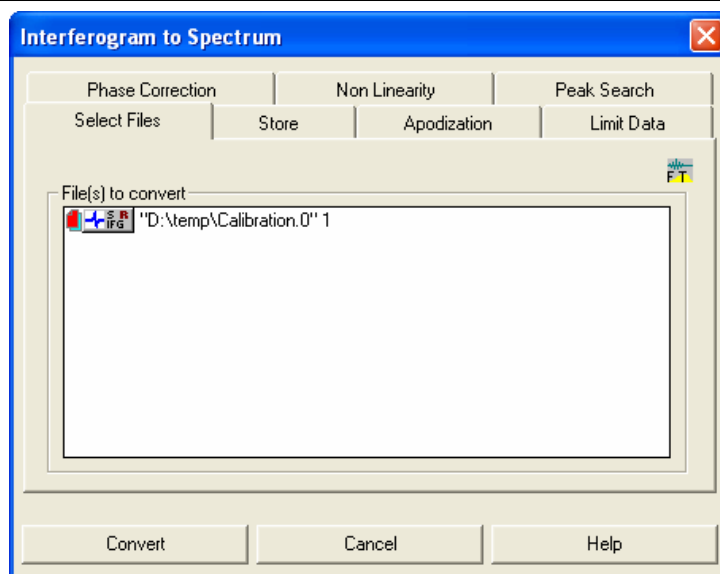
Fig.18: "Interferogram to Spectrum" dialog window - "Select files" page

- Click on the "Store". On this page you can choose the spectral range of the result spectrum. (See figure 19.) For polymer experiments, this is usually the fingerprint region. To be on the safe side, you can specify a somewhat broader spectral range as indicated in figure 19. It is extremely important that you activate the "Save phase" checkbox on the "Store" page. The resulting calibration phase spectrum of this "Interferogram to Spectrum" conversion will later be needed to evaluate the sample data. The power spectrum will not be needed, thus you do not have to activate the "Power" checkbox.
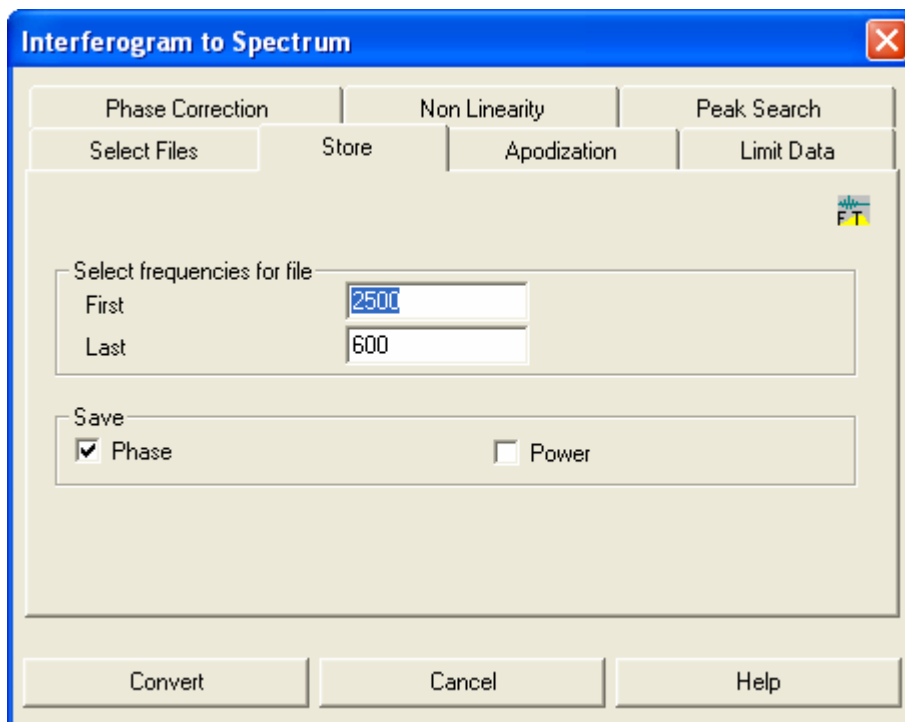
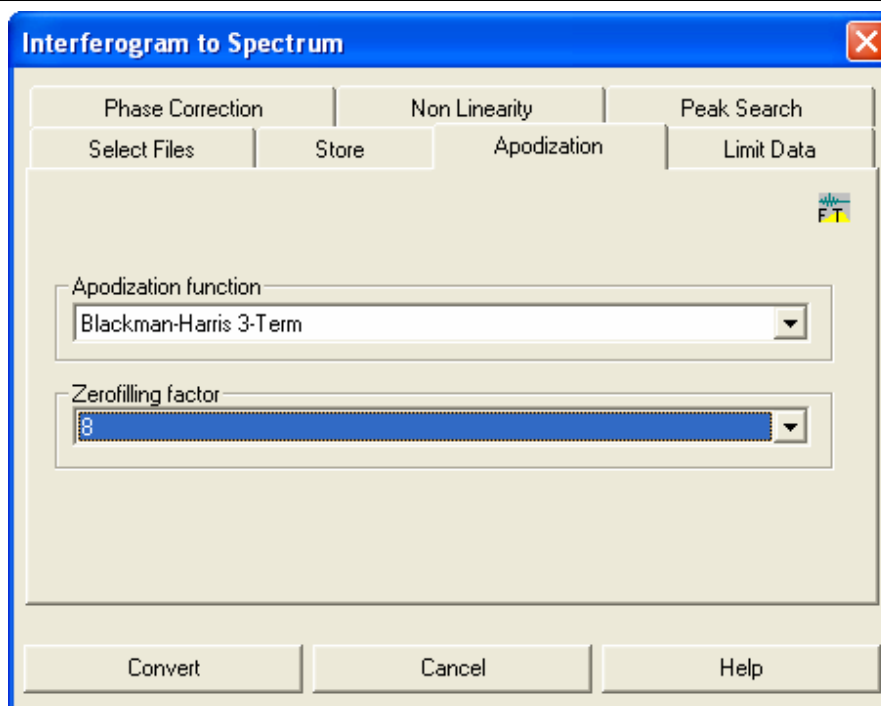**Fig. 19:** "Interferogram to Spectrum" dialog window - "Store" page

Fig. 20: "Interferogram to Spectrum" dialog window - "Apodization" page

- The parameters on the "Apodization" page (fig. 20) are identical to those on the corresponding page of the standard "Measurement" dialog window. The parameter settings shown in fig. 20 are useful for this kind of experiment, however, you can also try out other apodization functions and zerofilling factors.

- On the "Limit Data" page (fig. 21) the checkboxes "Limit resolution to" and "Limit phase resolution to" usually need not to be activated. Activate in the "Direction" group field the "Forward" option button and in the "Datapoints" group field the option button "Both". (See figure 21.)
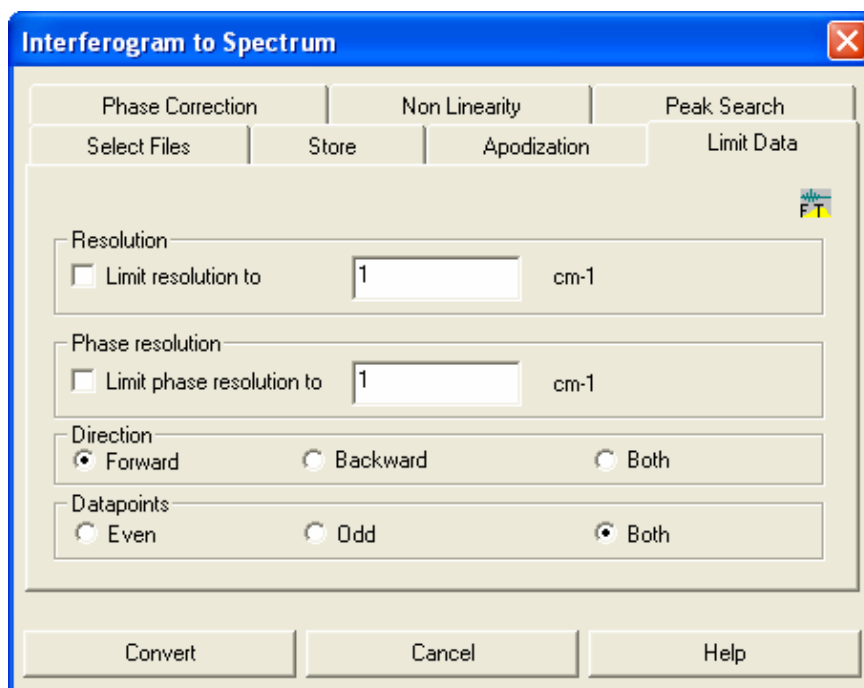

Fig. 21: "Interferogram to Spectrum" dialog window - "Limit Data" page

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- On the "Peak search" page, the peak search mode "Absolute largest value" and "Automatic" for the symmetry of the interferogram usually works fine as indicated in fig. 22. However, you can also fix the peak position (ZPD) to a particular value or optimize the position by entering a number larger than 0.
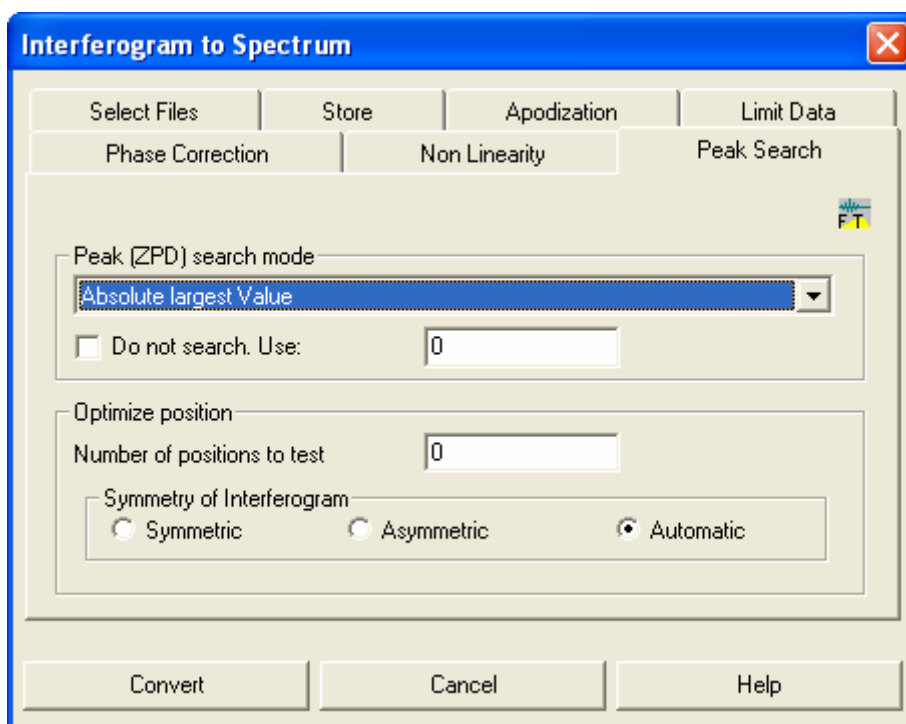

Fig. 22: "Interferogram to Spectrum" dialog window - "Peak Search" page

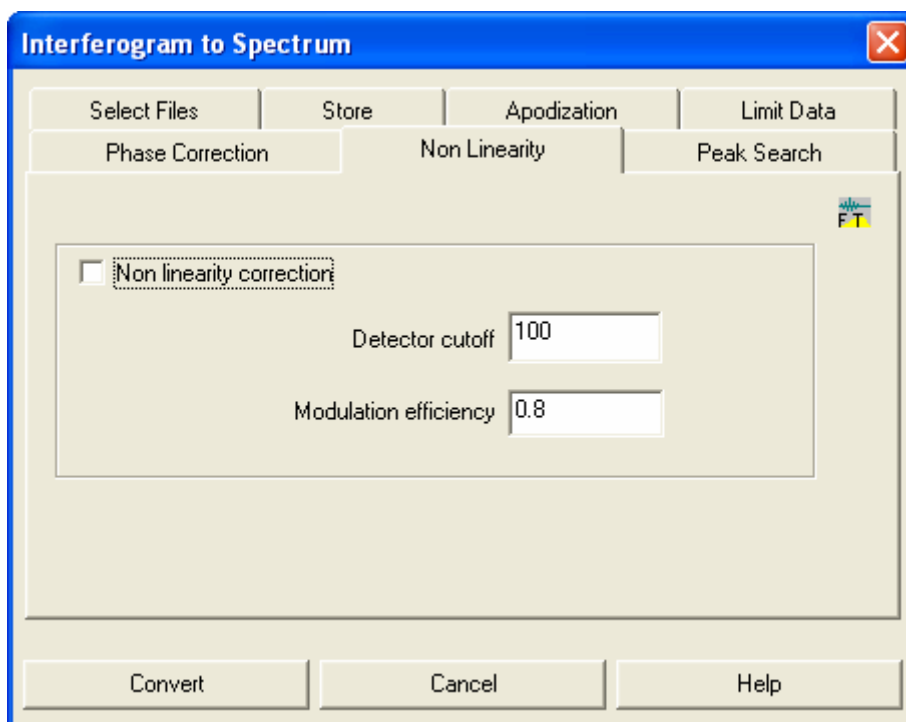- We recommend to do NO "non linearity correction" as shown in fig. 23.

Fig. 23: "Interferogram to Spectrum" dialog window - "Non Linearity" page

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- On the "Phase Correction" page, we recommend to choose the "Mertz" phase correction (fig. 24).
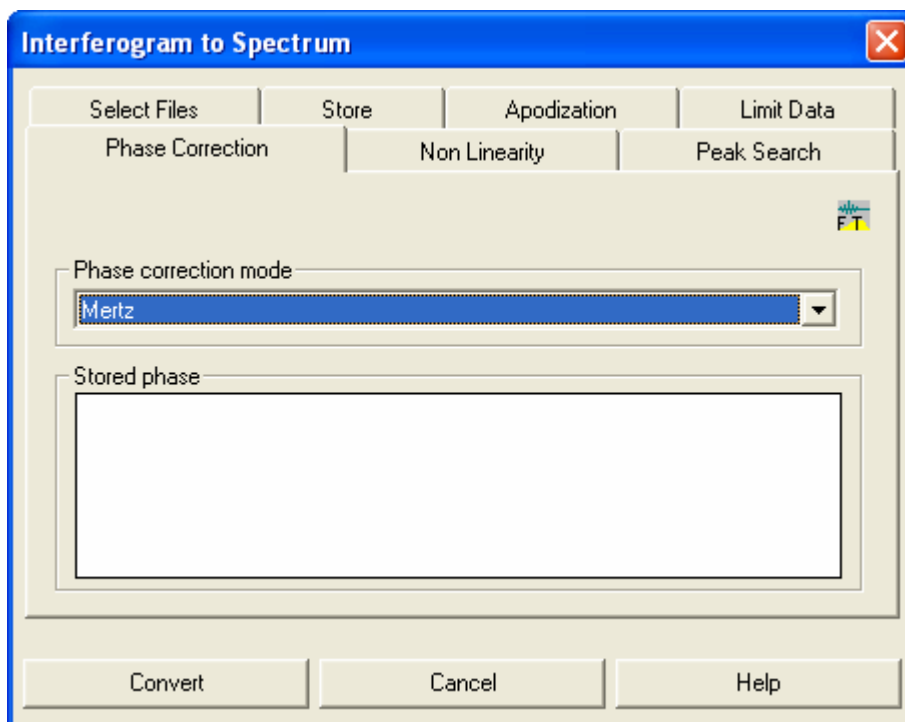

Fig. 24: "Interferogram to Spectrum" dialog window - "Non Linearity" page

- Click on the "Convert" button. As a result, two additional data blocks are added to the file resulting from the calibration measurement. The first data block **"SSC^R"** is the part of the single channel calibration spectrum which is in phase with the modulation. The second data block **"SPH^R"** is the phase spectrum which has been created by calculating the "SSC^R" spectrum. The phase spectrum "SPH^R" will be needed later in order to calculate the correct sample spectra.

5.3 Extraction of the constant part of the single channel sample spectrum

- Select the data block "IFG" of the file resulting from the sample measurement. This data block contains the part of the sample infrared signal which is independent from the modulation. Select in the "Manipulate" menu the "Interferogram to Spectrum" function. Thereupon, the "Interferogram to Spectrum" dialog window appears. (See figure 25.) This time, deactivate you "Save Phase" check box on the "Store" page. For the other parameters, use exactly the same settings as done before in case of the file resulting from the calibration measurement. Click on the "Convert" button. As a result, an additional data block **"SSC"** will be added to the file resulting from the sample measurement. (See figure 26). This file contains the constant part of the single channel sample spectrum which is independent from modulation.
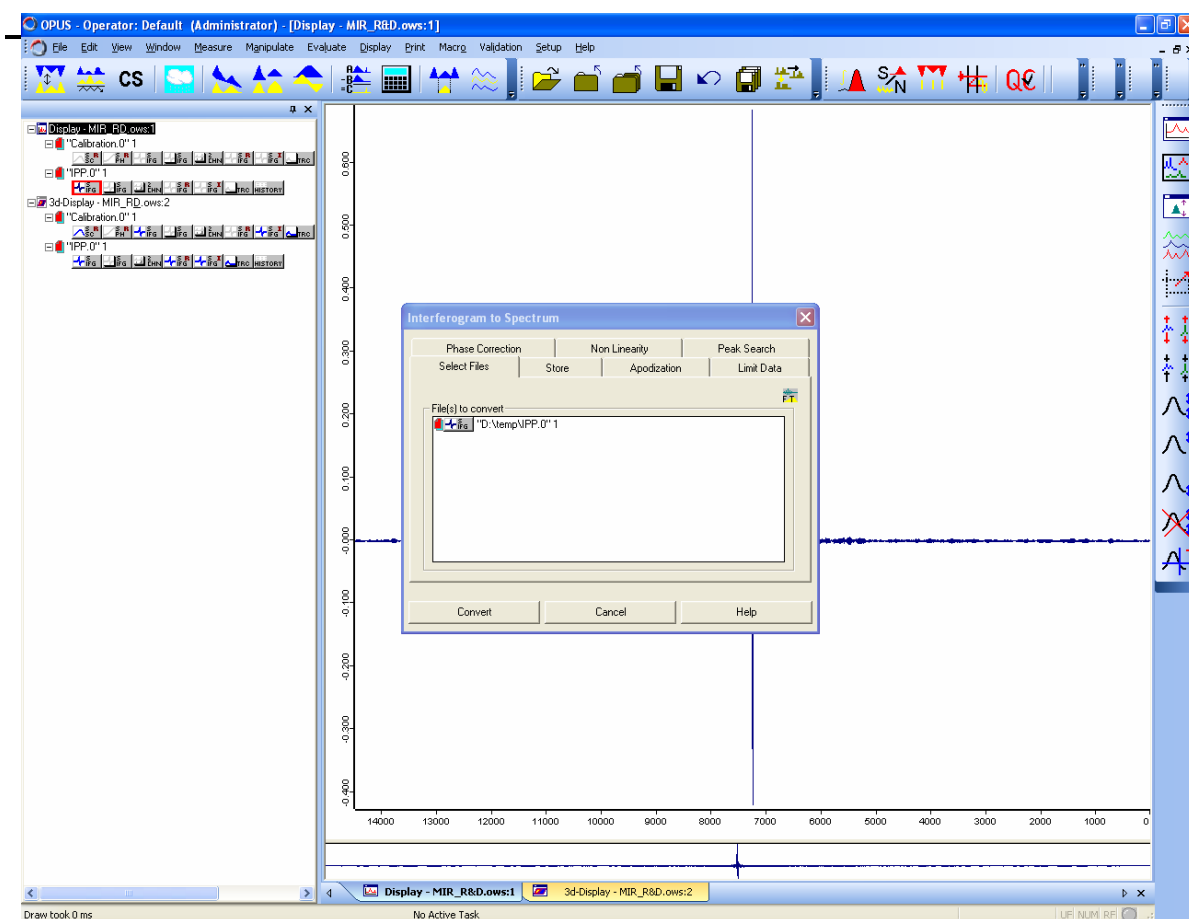
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Fig. 25: Appling the "Interferogram to Spectrum" function to the constant interferogram of the sample measurement
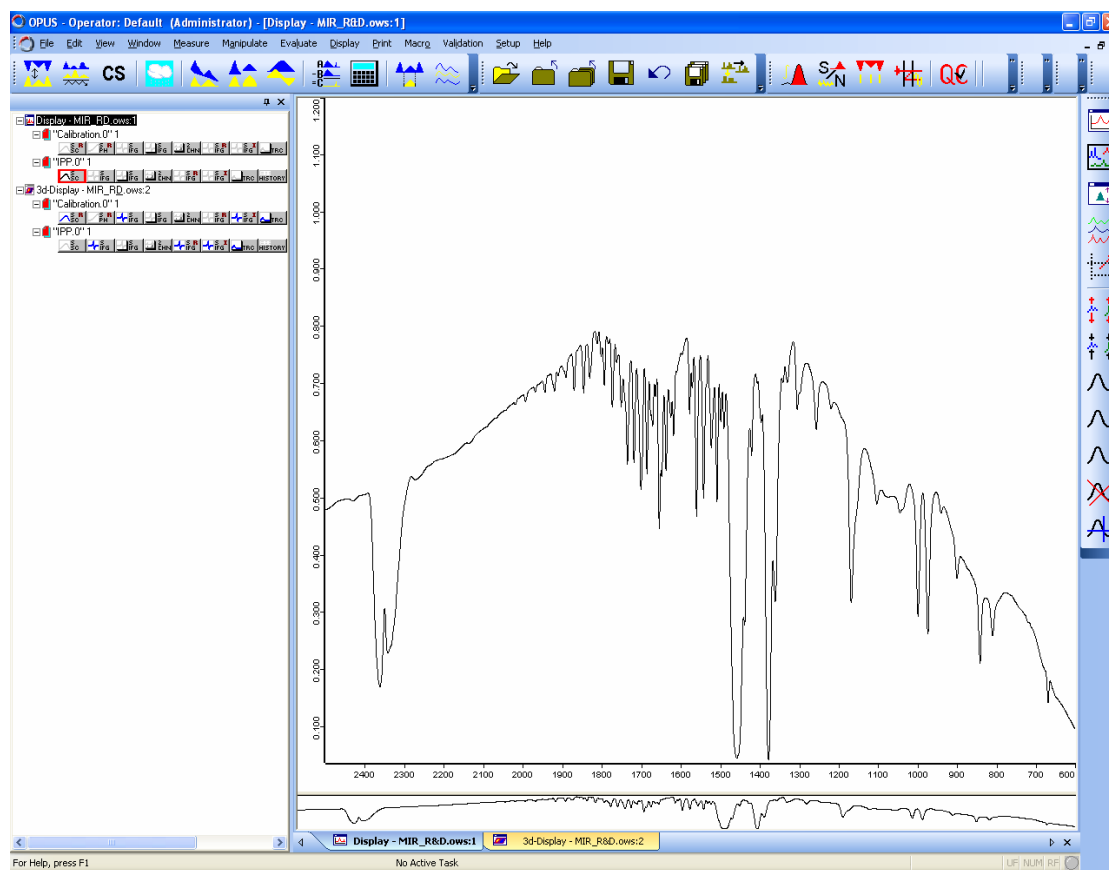
Fig. 26: Constant part of the single channel sample spectrum

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5.4 Calculation of the in-phase and out-of-phase single channel sample spectra

- This calculation is done once again using the "Interferogram to Spectrum" function, but for these signals, the calibration phase spectrum is used. By pressing the Ctrl button of the keyboard and using the mouse, select the data blocks "S_IFG^R" (the real part interferogram) and "S_IFG^I" (the imaginary part interferogram) of the file resulting from the sample measurement. Select in the "Manipulate" menu again the "Interferogram to Spectrum" function. Thereupon, the "Interferogram to Spectrum" dialog window appears. (See figure 27.)
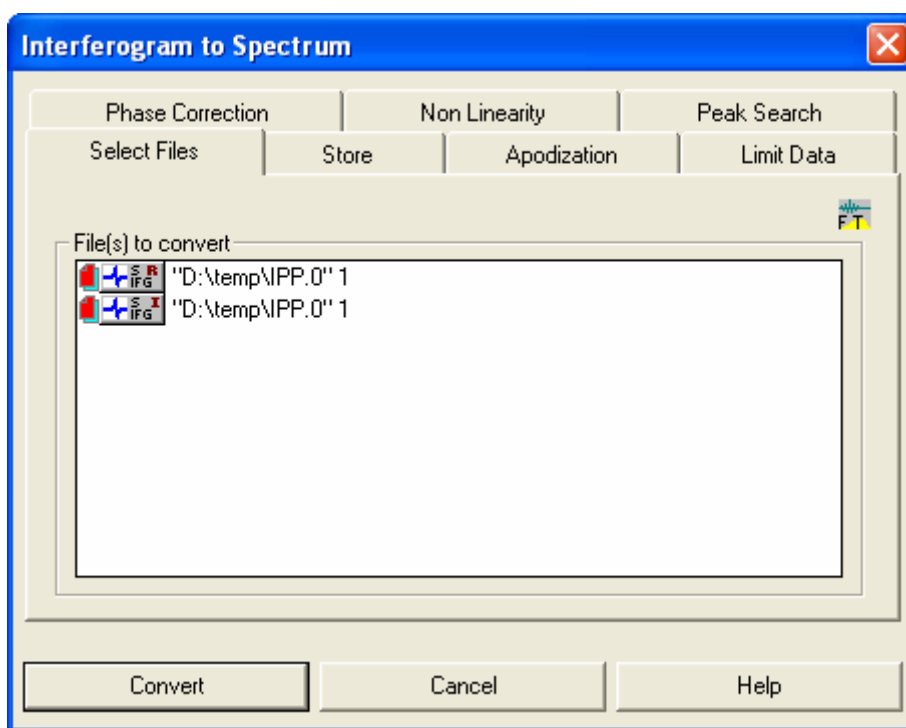
Fig. 27: Appling the "Interferogram to Spectrum" function to the real part sample interferogram and to the imaginary part sample interferogram

- Also for this conversion, do NOT store the phase (i.e. deactivate the "Save Phase" check box on the "Store" page). Click on the "Phase correction" tab. This time, select in the "Phase correction mode" drop-down list the option "Mertz/Stored Phase". Drag & drop the data block "SPH^R" (calibration phase spectrum) in the "Stored phase" field. (See figure 28.) All the other parameter settings have to be identical to the previous "Interferogram to Spectrum" conversions. Click on the "Convert" button. As a result, two additional data blocks are added to the file resulting from the sample measurement. The spectra of these data blocks are usually much smaller in intensity than the constant single channel sample spectrum. The data block **"SSC^R"** contains the in-phase single channel sample spectrum and the data block **"SSC^I"** contains the out-of-phase single channel sample spectrum.
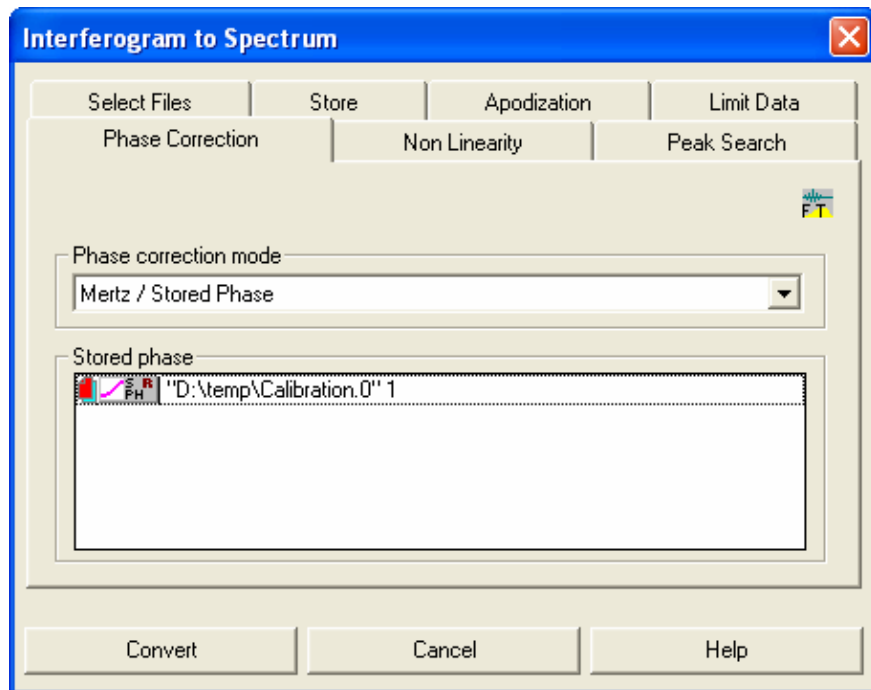
Fig. 28: Calibration phase spectrum in the "Stored phase" field.

5.5 Calculation of the in-phase and out-of-phase absorbance change spectra

- Click in the OPUS browser with the right mouse button on the file resulting from the sample measurement and copy the original file. (See figure 29).
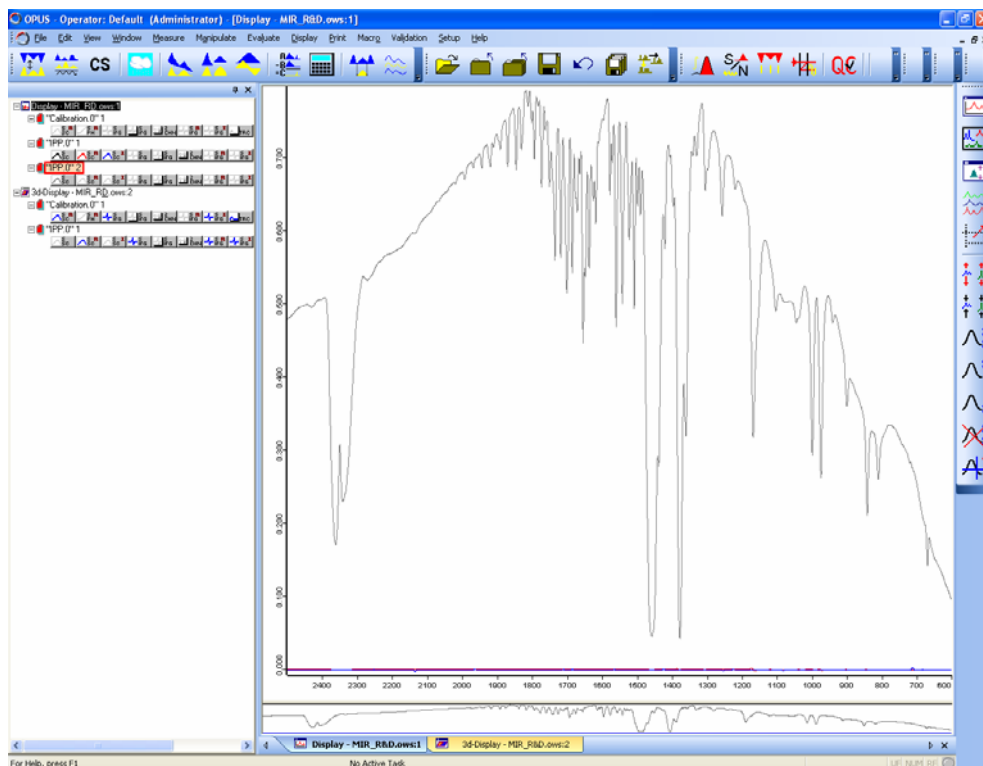

Fig. 29: Copying the entire sample measurement file with the "Copy Entry" function

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- Select in the "Manipulate" menu the "Spectrum Calculator" function. The in-phase absorption change (differential absorption) is calculated by dividing the in-phase single channel sample spectrum "SSC^R" by the constant single channel sample spectrum "SSC". Perform this calculation with the spectrum blocks of the original file resulting from the sample measurement:

In-phase absorbance change = "SSC^R" (sample) / "SSC" (sample)

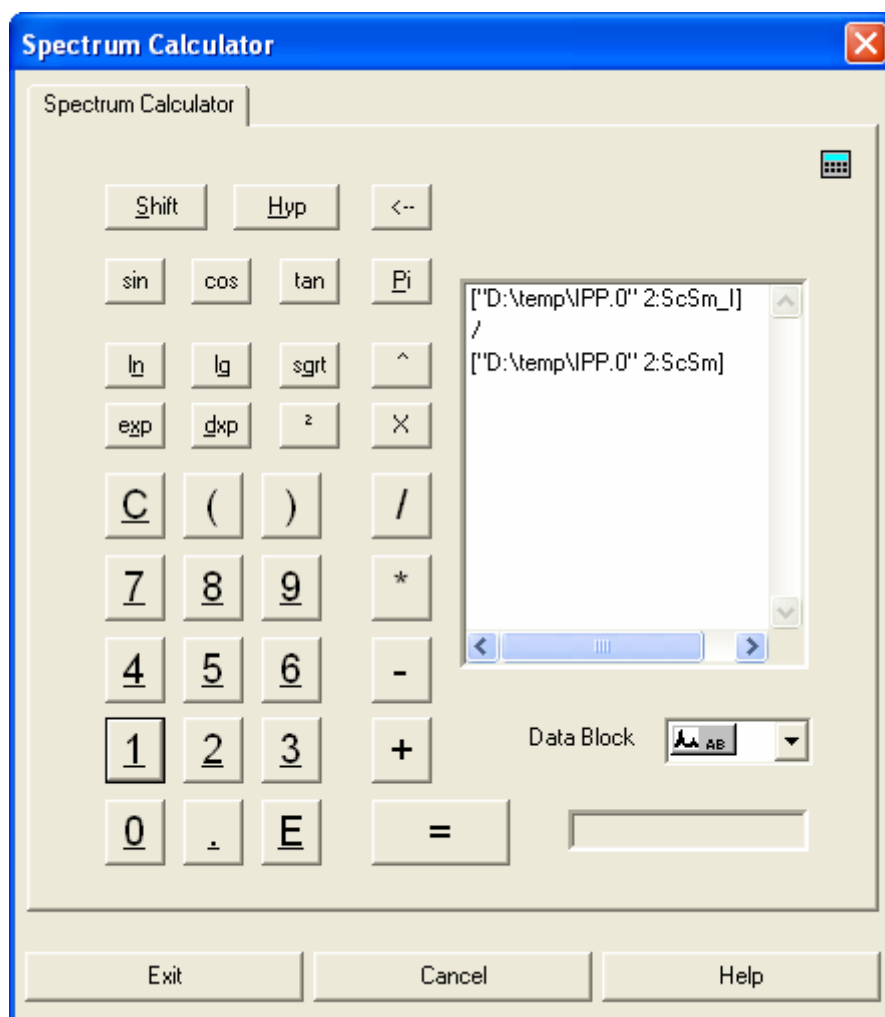Drag and drop the spectrum in the spectrum calculator. (See figure 30.)
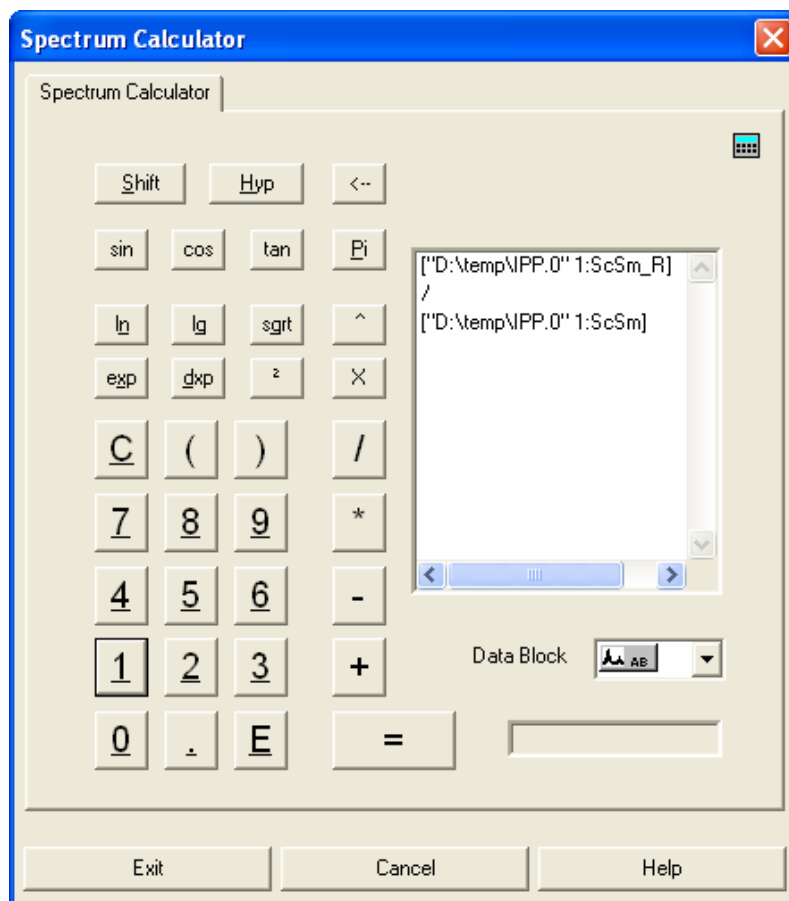
Fig. 30: Spectrum Calculator - Calculating the in-phase absorbance change of the sample

- Select in the spectrum calculator the absorbance data block and click on the "=" button.

- The out-of-phase absorbance change is calculated by dividing the out-of-phase single channel sample spectrum "SSC^I" by the constant single channel sample spectrum "SSC". Perform this calculation with the spectrum blocks of the copied file. (See figure 31.)

Out-of-phase absorption change = "SSC^I" (sample) / "SSC" (sample)

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Fig. 31: Spectrum Calculator – Calculating the in-phase absorbance change of the sample

After both types of absorbance changes have been calculated the evaluation is finished. Save the result spectra. Figure 32 shows the result.
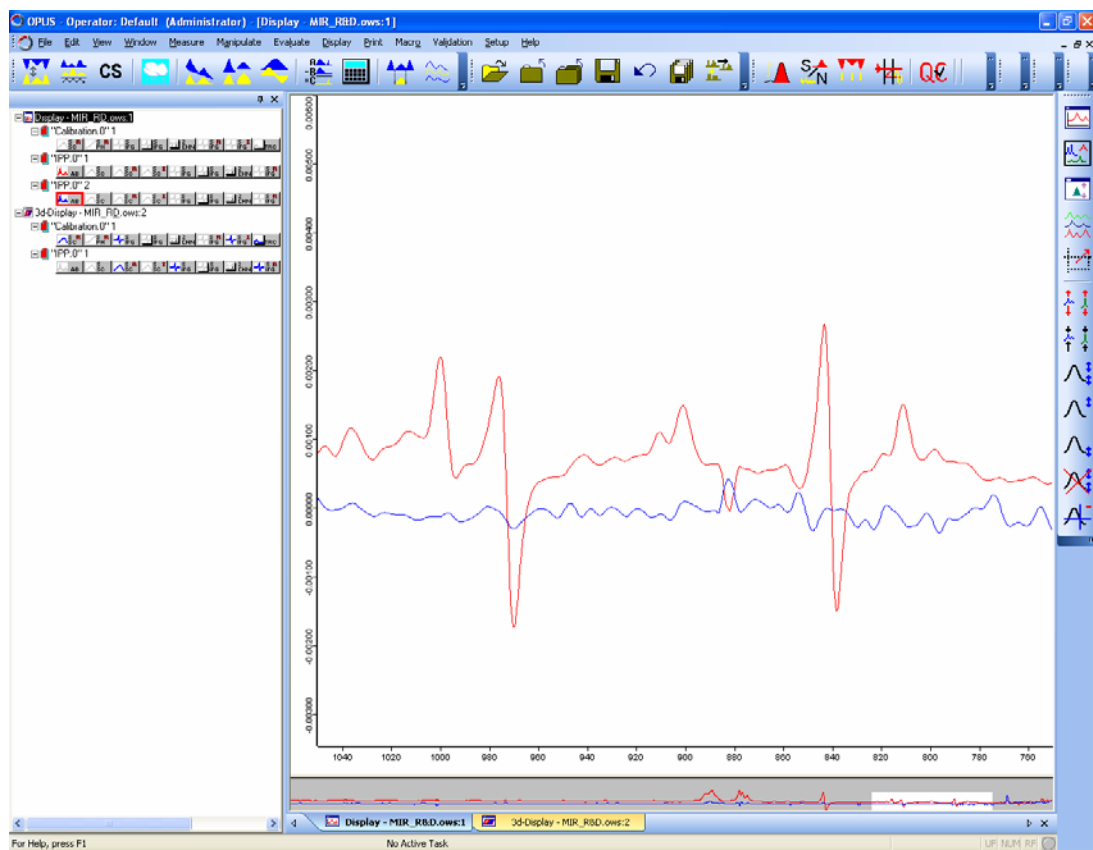
Fig. 32: In-phase (red) and out-of-phase (blue) absorbance change of the polymer sample

6. Appendix A – Safety Information

6.1 Warning labels

When operating the equipment you have to observe a number of safety instructions which are highlighted by various warning labels. This section describes the warning labels and explains their meaning. All warning labels on the equipment must always be kept legible. Immediately replace worn or damaged labels.

The following warning labels indicate different dangerous situations which may be caused by improper use of the equipment.

Caution – General Hazard
the precautions described to avoid personal injury and/or property damage.

Caution – Electric Shock
This warning symbol indicates electrical hazard. This symbol is located near live parts or on enclosures behind which are live parts that represent an accidental contact hazard. Never touch these parts. Before removing the corresponding compartment covers and beginning any maintenance or repair work, first turn off the main power switch and unplug the main power cable. Ensure that all live parts do not come into contact with a conductive substance or liquid. Non-observance of these safety instructions can cause severe personal injury and/or property damage.

Caution – Hot Surface
This warning symbol refers to components and surfaces which can become very hot during operation. Do not touch these components and surfaces. Risk of skin burn! Be careful when operating near hot components and/or surfaces.

Caution – Frostbite
This warning symbol indicates the existence of cryogenic materials (e.g. liquid nitrogen) required to operate the module (e.g. cooling detector). Skin contact with these liquids or cooled components causes severe frostbite. Always handle the liquids with utmost care. Observe the safety instructions for handling of cryogenic liquids.

Caution – Harmful or Irritant Material
This warning label indicates the existence of harmful or irritant material (e.g. ZnSe window material). Observe the safety instructions on the packaging, and the safety data sheets attached. Non-observance may cause severe personal injury or even death.

Caution Toxic Material
This warning label indicates the existence of toxic material (e.g. KRS-5 material). Observe the safety instructions on the packaging, and the safety data sheet attached. Non-observance may cause severe personal injury or even death.

Beside the dangers described above, there can also be hazards caused by the sample material. Depending on the type of hazardous substances used, you have to observe the specific substance-relevant safety instructions. Put on the specific warning label on the corresponding module position. The label must be legible and permanently discernible. The following list exemplifies types of hazardous substances:

Caution – Infectious Material

This warning symbol indicates the possible existence of biologically dangerous and infectious material. When working with this kind of material always observe the prevailing laboratory safety regulations and take necessary precautions and disinfection measures (e.g. wearing protective clothing, masks, gloves etc.). Non-observance may cause severe personal injury or even death.

 (For information on how to use, dilute and efficiently apply disinfectants, refer to the *Laboratory Biosafety Manual:* 1984 by WHO – World Health Organisation)

Caution – Radioactive Material

This warning symbol indicates the possible existence of radioactivity. When working with radioactive material always observe the safety regulations and take necessary protective measures. Wear protective clothing, e.g. masks and gloves. Non-observance may cause severe personal injury or even death.

Caution – Corrosive Substance

This warning symbol indicates the possible existence of corrosive substances. When working with corrosive substances always observe the laboratory safety regulations, and take protective measures (e.g. wear protective masks and gloves). Non-observance may cause severe personal injury or even death.

6.2 Waste disposal

Dispose all waste produced (chemical, infectious and radioactively contaminated substances etc.) according to the prevailing laboratory regulations. Detergents and cleaning agents must be disposed according to the special waste regulations.

7. Appendix B – Service Addresses

Bruker Optik has an international network of branch offices and representations to ensure a competent customer service throughout the world. The following list includes the addresses of Bruker headquarters.
For a complete list with the addresses and telephone numbers of the Bruker branch offices and representations worldwide, refer to the internet:

http://www. brukeroptics.com/contacts/worldwide.html

North America
Bruker Optics Inc
19 Fortune Drive, Manning Park
Billerica, MA 01821 - 3991
USA
Phone: +1 978 439 9899 (ext. 5227)
Fax: +1 978 663 9177
www.brukeroptics.com
info@brukeroptics.com

Europe
Bruker Optik GmbH
Rudolf-Plank-Str. 27
76275 Ettlingen
Germany
Phone: +49 7243 504 619/600
Fax: +49 7243 504 698
www.brukeroptics.de
info@brukeroptics.de

Asia
Bruker Optik Asia Pacific Ltd.
Unit 601, 6/F, Tower 1
Enterprise Square
No. 9, Sheung Yuet Road
Hong Kong
Phone: +852 2796 6100
Fax: +852 2796 6109
asiapacific@brukeroptics.com.hk

No responsibility can be taken for the correctness of this information. Subject to changes.